PB85-204360

Master Analytical Scheme for Organic Compounds in Water. Part 2 Appendices to Protocols

Research Triangle Inst.
Research Triangle Park, NC

Prepared for

Environmental Research Lab., Athens, GA

Jan 85

U.S. Department of Commerce
National Technical Information Service
NTIS

PB85-204360

EPA/600/4-84/010b
January 1985

MASTER ANALYTICAL SCHEME FOR ORGANIC COMPOUNDS IN WATER

PART 2. APPENDICES TO PROTOCOLS

by

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Contract No. 68-03-2704

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U.S. Environmental Protection Agency
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ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GA 30613

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TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/4-84/010b	2.	3. RECIPIENT'S ACCESSION NO. PB85 204360/AS
4. TITLE AND SUBTITLE Master Analytical Scheme for Organic Compounds in Water: Part 2. Appendices to Protocols		5. REPORT DATE January 1985 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) E.D. Pellizzari, L.S. Sheldon, J.T. Bursey, L.C. Michael and R.A. Zweidinger		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Research Triangle Institute P.O. Box 12194 Research Triangle Park NC 27709		10. PROGRAM ELEMENT NO. ABWD1A 11. CONTRACT/GRANT NO. 68-03-2704
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency--Athens GA Office of Research and Development Environmental Research Laboratory Athens GA 30613		13. TYPE OF REPORT AND PERIOD COVERED Final, 9/78-7/83 14. SPONSORING AGENCY CODE EPA/600/01

15. SUPPLEMENTARY NOTES

Part 1: Protocols, EPA/600/4-84/010a

microgram/

16. ABSTRACT

A Master Analytical Scheme (MAS) has been developed for the analysis of volatile (gas chromatographable) organic compounds in water. In developing the MAS, it was necessary to evaluate and modify existing analysis procedures and develop new techniques to produce protocols that provide for the comprehensive qualitative-quantitative analysis of almost all volatile organics in many types of water. The MAS provides for analysis of purgeable and extractable, as well as neutral and ionic water soluble, organics in surface and drinking waters and in leachates and various effluents. Nominal lower quantifiable limits range from 0.1 μg/L to 100 μg/L, depending on chemical/physical class of the analyte and complexity of the aqueous matrix. Recoveries are reported for about 280 model compounds of a wide variety of chemical classes and physical properties dosed into representative samples of several major types of water. The appendices include specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, computerized relative molar response and recovery data for standards and analytes, and documentation of the MASQUANT computer program for quantification of MAS data.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 239
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (9-73)

DISCLAIMER

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FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific contaminants in the envrionment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of envrironmental contaminants, the Analytical Chemistry Branch characterizes chemical constituents of water and soil.

Chemists working in governmental, industrial, and academic laboratories have long recognized a need for a comprehensive analytical methodology for organic compounds in water. To this end, research was begun in 1978 to develop a qualitative-quantitative scheme for the analysis of organics of all volatility classes (amenable to gas chromatography), of almost all functional groups, in almost any water sample. The result is the Master Analytical Scheme (MAS) for Organic Compounds in Water, a compilation of protocols that employ new techniques and modifications of existing analysis procedures. Users may apply the MAS as a set of protocols for a comprehensive analysis or use individual protocols separately for analysis of organic fractions of particular interest. Among its many applications are epidemiological studies, wasteload allocations, permit application evaluations, trends analyses, watershed management studies, exposure assessments, landfill hazard evaluations, and aqueous source characterizations.

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Director
Environmental Research Laboratory
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PREFACE

The Master Analytical Scheme (MAS) represents the first effort to develop a comprehensive qualitative-quantitative scheme for the analysis of organic compounds in water. The MAS is a set of analytical protocols that includes a broad scope of organics with a wide variety of functional groups and physical properties. These protocols provide for the GC/MS/computer analysis of the usual purgeable and extractable compounds, with the addition of various neutral and ionic water soluble compounds; in fact, the MAS is applicable to any compound that can pass unchanged through a gas chromatograph, or can be derivatized to do so. Recoveries have been determined from distilled and drinking water, industrial and municipal effluents, and, in some cases, surface water and energy effluents, so the protocols are expected to be applicable to most water types. One unique feature of the MAS is its comprehensiveness. Another is its qualitative-quantitative aspect: an extensive data base of mass spectrometer detector response and recovery factors allows computer estimation of concentration without recourse to standards for each analyte.

In developing the MAS, existing analytical techniques were evaluated and modified and new techniques were developed to produce the comprehensive protocols. Development was in two stages. An interim set of protocols was developed by October 1980; analysis of environmental samples by these protocols revealed several important deficiencies that were subsequently corrected by additional experimental work. The final result is this first edition of MAS protocols in two parts; this volume, Part 2, contains the Appendices.

Two companion reports resulted from MAS development: Experimental Development of the MAS for Organic Compounds in Water, and Literature Review for Development of the MAS for Organic Compounds in Water. The user can refer to the experimental development report for information on techniques considered for MAS incorporation and experiments dealing with technique optimization and recovery studies. The literature review, which covers material through June 1982 on techniques for analysis of organics in water, was the starting point for experimental development, and will also be of interest to many users. Neither companion report is essential to MAS use, however; this report (Part 1: Protocols and Part 2: Appendices to Protocols) stands alone as the handbook for implementation. Part 2 includes: Appendix A - specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, Appendix B - hard copy of computerized relative molar response and recovery data for standards and analytes, and Appendix C - documentation of the MASQUANT computer program for quantification of MAS data.

The prospective MAS user should first thoroughly familiarize himself with Chapters 1 and 13 (the Introduction and GC-MS-COMP Analysis Procedures) of Part 1 of this report for an overview and a guide to use of the protocols and these appendices.

ABSTRACT

A Master Analytical Scheme (MAS) has been been developed for the analysis of volatile (gas chromatographable organic compounds in water. In developing the MAS, it was necessary to evaluate and modify existing analysis procedures and develop new techniques to produce protocols that provide for the comprehensive quantitative-qualitative analysis of almost all volatile organics in manytypes of water. The MAS provides for analysis of purgeable and extractable, as well as neutral and ionic water soluble, organics in surface and drinking waters and in leachates and various effluents. Nominal lower quantifiable limits range from 0.1 μg/L to 100 μg/L, depending on chemical/physical class of the analyte and complexity of the aqueous matrix. Recoveries are reported for about 280 model compounds of a wide variety of chemical classes and physical properties dosed into representative samples of several major types of water. The appendices include specific instructions on fabrication of the purge and trap apparatus and ancillary devices for purgeable organics, computerized relative nolar response and recovery data for standards and analytes, and documentation of the MASQUANT computer program for quantification of MAS data.

This report was submitted in fulfillment of Contract No. 68-03-2704 by Research Triangle Institute under the sponsorship of the U.S. Environmental Protection Agency. This report covers the period from September 1978 to July 1983, and work was completed as of July 1983.

CONTENTS

Appendices

A Fabrication of Purge and Trap Apparatus and Ancillary Devices. 1

B RMR and Recovery Data File for Internal and External Standards and Analytes in MASQUANT 24

C Description of Computer Program MASQUANT for Processing Data Collected Using MAS 184

APPENDIX A

FABRICATION OF PURGE AND TRAP APPARATUS AND ANCILLARY DEVICES

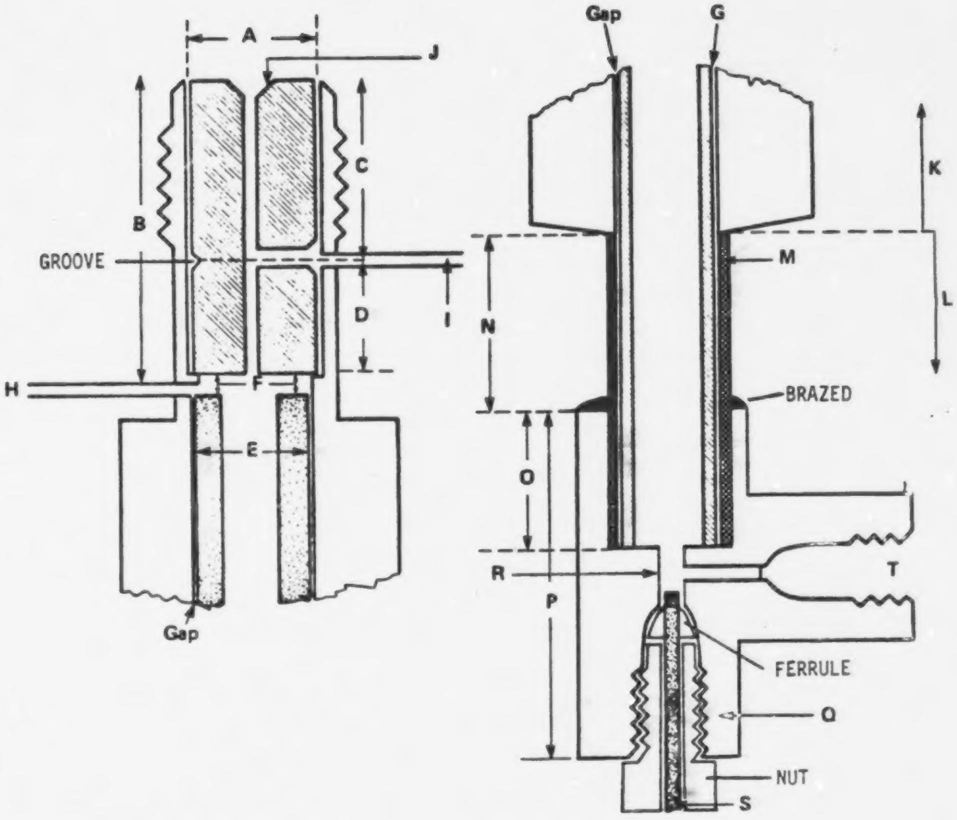
INTRODUCTION

This appendix describes the fabrication of a purge and trap device, an injection port/cryofocussing module, and other ancillary devices for use with the protocols for analysis of volatile organics, VO (Chapter 6), and neutral water soluble low molecular weight compounds, NEWS (Chapter 7). Most of the listed components are commercially available and, where necessary, the fabrication of devices can be easily performed by machine and glass blowing shops. Materials and machine and glass blowing shop labor are estimated to cost approximately $4,000.00.

FABRICATION OF INJECTION PORT

The features of this injection system include the capability for; (1) introduction of VO compounds for the determination of mass spectrometric relative molar response factors; (2) introduction of system performance mixtures; and (3) addition of an external standard (perfluorotoluene) with each water sample analyzed for VO and NEWS compounds and for RMR determinations.

Figure A-1 shows the construction of the injector body. An on-column flash vaporizer packed column injector (Varian Model 1040) is drilled out to 7.5 mm i.d. (A), to a depth of 15 mm. From there, the original 6.4 mm (1/4") i.d. is maintained, forming a lip at a 15 mm depth. Two 1.6 mm (1/16") o.d., 1.0 mm (0.040") i.d. stainless steel tubes are brazed onto the injector body: the carrier gas inlet (H) about 1 mm below the lip (16 mm below the top) on the same side of the injector as the original carrier gas inlet and the septum flush outlet (I) 10 mm below the top just beneath the septum nut threads. The septum flush outlet is attached on the opposite side of the injector body from the carrier inlet. A 1.6 mm (1/16") stainless steel zero dead volume tee (Q, Perkin Elmer No. 0091291) is modified to make the splitter. To minimize dead volume between the glass insert and the splitter outlet, the top of the tee is drilled out (O) to accommodate a piece of 6.4 mm (1/4") i.d. stainless steel tubing (M) 23 mm long (o.d. is not critical), the tee and tubing are brazed together. The bottom of the injector is cut off immediately below the


Gap
G
A
J
B
C
K
GROOVE
M
D
I
N
L
H
F
BRAZED
E
O
R
T
P
FERRULE
Q
NUT
S
Gap

(A) 7.5 mm i.d.; (B) 16mm; (C) 10 mm; (D) 5 mm; (E) 6.35 mm o.d. glass tube; (F) 2-3 mm; (G) 6.35 mm glass tube; (H) carrier gas inlet (1/16" o.d. SS tubing); (I) septum purge outlet (1/16" o.d. SS tubing connected to Hoke #1315G2B needle valve); (J) beveled needle guide into stainless steel insert with 1.6 mm i.d. hole; (K) old injector body; (L) new materials; (M) 6.4 mm (1/4") i.d. SS tubing; (N) 13 mm; (O) 10 mm; (P) 24 mm; (Q) zero dead volume SS Tee; (R) 1.2 mm i.d.; (S) Ni capillary tubing; (T) splitter outlet (1.6 mm fitting connected to Hoke #1315G2B needle valve).

Figure A-1. Diagram of injector body.

hexagonal block and the other end of the 6.4 mm i.d. tube connected such that the top of the tee is about 13 mm below the injector body (N). Care must be taken to ensure that these connections, both of which are brazed, are properly aligned. We have found that using a lathe to cut a concentric lip into the bottom of the injector body to accommodate the space tube aids in the alignment process.

The stainless steel insert (J) for the top of the injector has an i.d. of 1.6 mm. The o.d., about 7.1 mm, is matched with 7.5 mm i.d. of the upper part of the injector body (A) such that the fit is close, but not binding. The insert is about 14.5-15 mm long such that the septum will be tightened down snugly over the top. A 1.6 mm (1/16") hole is drilled in one side at about 10 mm from the top (C), even with the septum purge outlet (I). A groove is cut around the insert at the 1.6 mm outlet hole. The top of the insert hole (of J) is beveled to act as a needle guide.

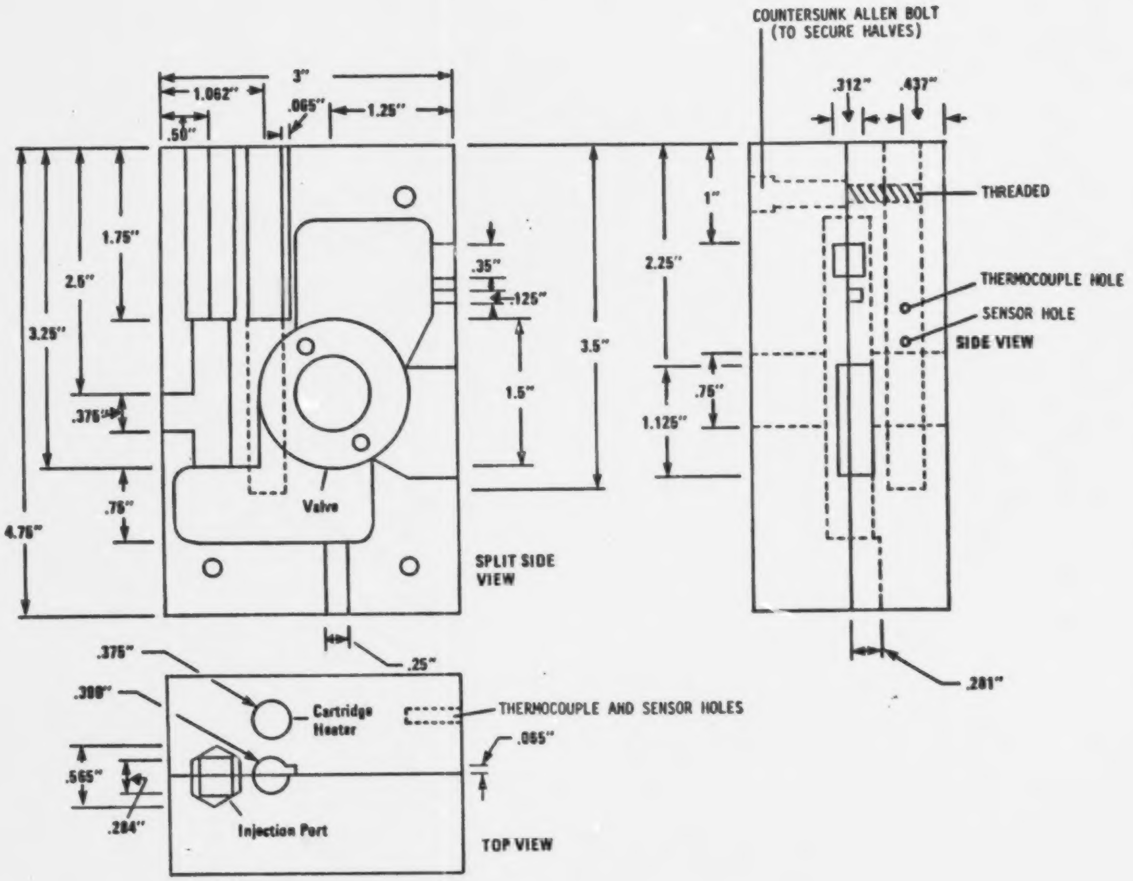
Glass inserts are fabricated from standard 6.35 mm o.d. Pyrex tubing about 7 cm in length such that there is a 2 mm gap between the top of the glass and the bottom of the stainless steel septum purge insert.

The injector is installed in a heating block which also is fabricated to accommodate the six-port high temperature Valco valve. The septum purge outlet (I) is attached to a needle valve (Hoke #1315G2B) and then to vent. The splitter outlet (T) is connected to another needle valve. A shutoff valve (e.g., Whitey SS-OGS2) may also be added for operation in the "splitless" mode, and after the needle valve on the septum purge for shutoff of the purge.

Glass inserts for the injector are easily fabricated from standard 6.35 mm o.d. column tubing of 2-4 mm i.d.; inserts are silanized with dimethylchlorosilane. Replacement in the injector requires approximately 30 sec.

FABRICATION OF HEATING BLOCK AND CRYOTRAP

An aluminum heating sandwich is machined according to the specifications in Figure A-2.



COUNTERSUNK ALLEN BOLT
(TO SECURE HALVES)
3"
1.062"
.50"
.065"
1.25"
1.75"
2.5"
3.25"
.375"
.75"
4.75"
.35"
.125"
1.5"
3.5"
Valve
SPLIT SIDE VIEW
.312"
.437"
1"
2.25"
.75"
1.125"
THREADED
THERMOCOUPLE HOLE
SENSOR HOLE
SIDE VIEW
.281"
.25"
.375"
.388"
Cartridge Heater
THERMOCOUPLE AND SENSOR HOLES
.065"
.565"
.284"
Injection Port
TOP VIEW

Figure A-2. Specification of heating block (see Fig. A-4).

A cryotrap is fabricated according to the dimensions given in Figure A-3. An aluminum rod (1.9 cm O.D. × 4.0 cm in length) is bored (1.6 cm I.D.) to a depth of 1.5 inches to accept a 150 watt heating cartridge (Table A-1). A helical groove (one-half the diameter of the Ni capillary) is machined around the aluminum cylinder to accept a nickel capillary trap with the dimensions shown in Figure A-3. Also, a groove is made to provide for the return end of the trap (B, Fig. A-3). Two additional grooves are machined (the thicknesses of the thermocouples must be measured for determining width and depth of the grooves; thermocouples should fit snugly) for the controller and sensor thermocouples. An aluminum cup is machined according to the specifications given in Figure A-3 so that it fits snugly over the outside of the capillary trap when it is wrapped on the aluminum cylinder. The aluminum cup is 2 cm deep. The thermocouples are inserted between the capillary trap and the aluminum cylinder at the approximate positions shown in Figure A-3. A 1/16 in Swagelock® union is fastened into the threaded hole of the aluminum cup to provide for filling of the cup with liquid nitrogen during the cryofocussing step.

The injection port system is assembled as shown in Figure A-4. The 1/16 in Ni sample transfer line from the purge and trap system is attached as indicated to the Valco® valve (Fig. A-4, A). All lines are connected so that the flow pattern through the valve and cryotrap are as indicated in Figure A-5 (for valve position A and B). (It is extremely important that the direction of gas flow through the cryotrap is the same for valve position A and B.) Nickel tubing (1/16 in OD, 0.02 in ID) is used for connecting the injector to the Valco® valve (A) and the valve to the 1/16 in zero dead volume Swagelock® union (Fig. A-4, B). The fused silica capillary is passed through the commercial GC injection port and connected flush to the constricted part of B using a graphite ferrule. The injection port system must be secured (bolted) to the commercial GC system to provide stability during usage. The entire assembly (Fig. A-4) is fastened flush with the commercial GC injection port.

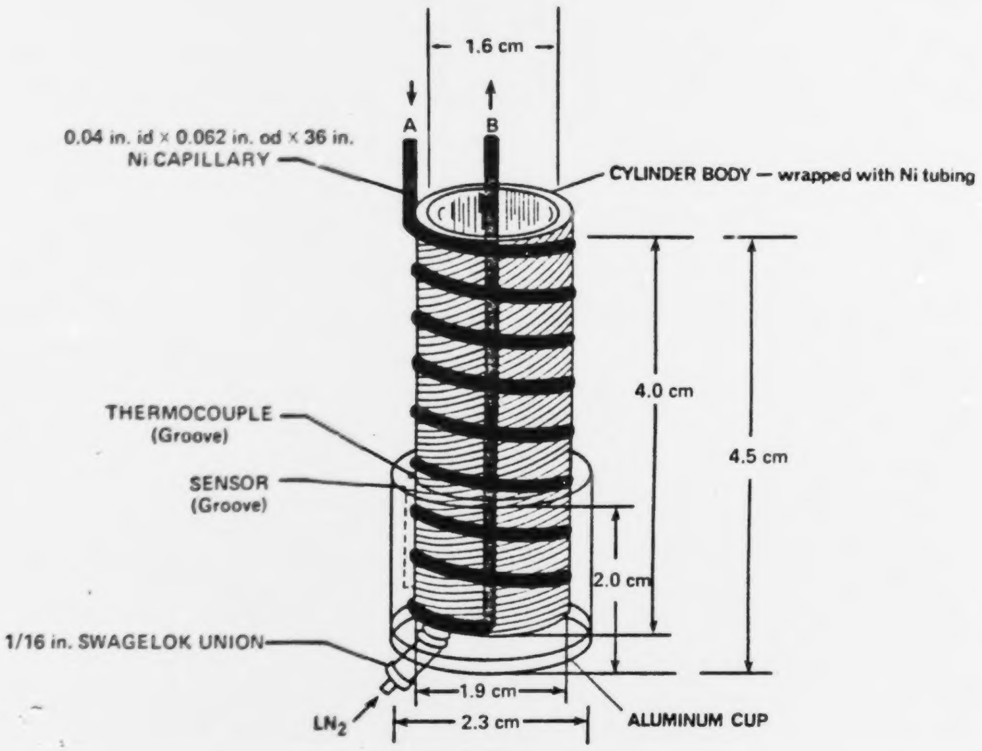

1.6 cm
A
B
0.04 in. id × 0.062 in. od × 36 in.
Ni CAPILLARY
CYLINDER BODY — wrapped with Ni tubing
4.0 cm
4.5 cm
THERMOCOUPLE
(Groove)
SENSOR
(Groove)
2.0 cm
1/16 in. SWAGELOK UNION
1.9 cm
2.3 cm
LN$_2$
ALUMINUM CUP

Figure A-3. Diagram of cryofocussing trap.

Table A-1. PARTS LISTING FOR TEMPERATURE CONTROLLERS

Quantity	Manufacturer	Part Number	Description
CONNECTORS			
2	Molex	receptacle 03-09-1091, plug 03-09-2091	9 circuit
2	Molex	receptable 03-09-1061, plug 03-09-2061	6 circuit
2	Molex	receptacle 03-09-1031, plug 03-09-2031	3 circuit
2	Molex	receptacle 03-09-1021, plug 03-09-2021	2 circuit
8	Omega	mated pair NMP-IRCO-MF	miniature thermocouple connectors for type J
MISCELLANEOUS			
	Molex	.093" Pin terminals for above Molex connectors	
40	Molex	02-09-1118 Female	
40	Molex	09-09-2118 Female	
8	Omega	MACL pnael adaptor clips	
2	Omega	Model 7035-J-500 meter; 0-260≥C, I/C type J thermocouple	
2	CentraLab	PA-2003 Rotary switch; 6 position non-shorting	
-	Omega	28AWG Thermocouple wire for read out	
2	Littlefuse	3AMP 3AG 312 Fuse	
6	Littlefuse	2AMP 3AG 312 Fuse	
8	Buss	Type HTA fuse holders, panel mount	
8	McGill	Toggle switch SPST No. 90-0003	
CONTROLLERS			
6	Wattlow	Series 100 Temperature controller with type J thermocouples	
HEATERS			
6	Hotwatt	GR16-60	Single rope heater 250 watt, 60" long
1	Hotwatt	HS3715	Cartridge heater 150 watt, 1.5" long
1	Hotwatt	HS3725	Cartridge heater 200 watt, 2.5" long

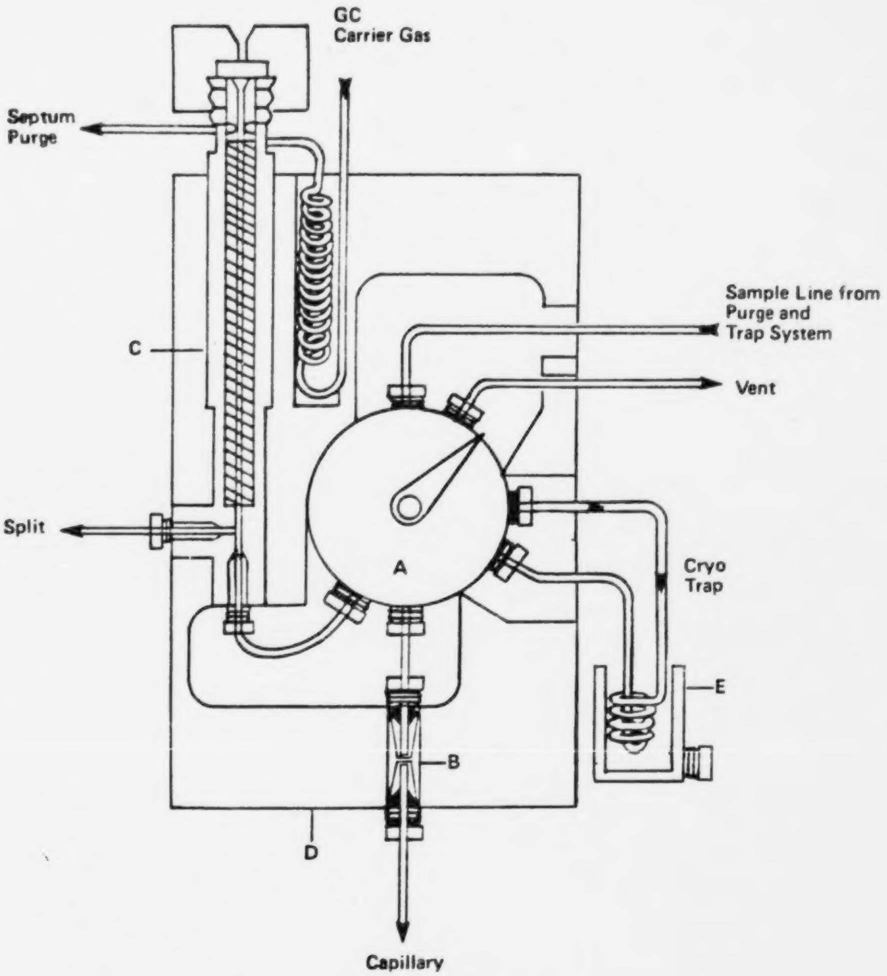

GC
Carrier Gas
Septum
Purge
Sample Line from
Purge and
Trap System
C
Vent
Split
Cryo
Trap
A
E
B
D
Capillary

Figure A-4. Diagram of heating block (D) with injector (C), Valco valve (A), and cryofocussing trap (E).

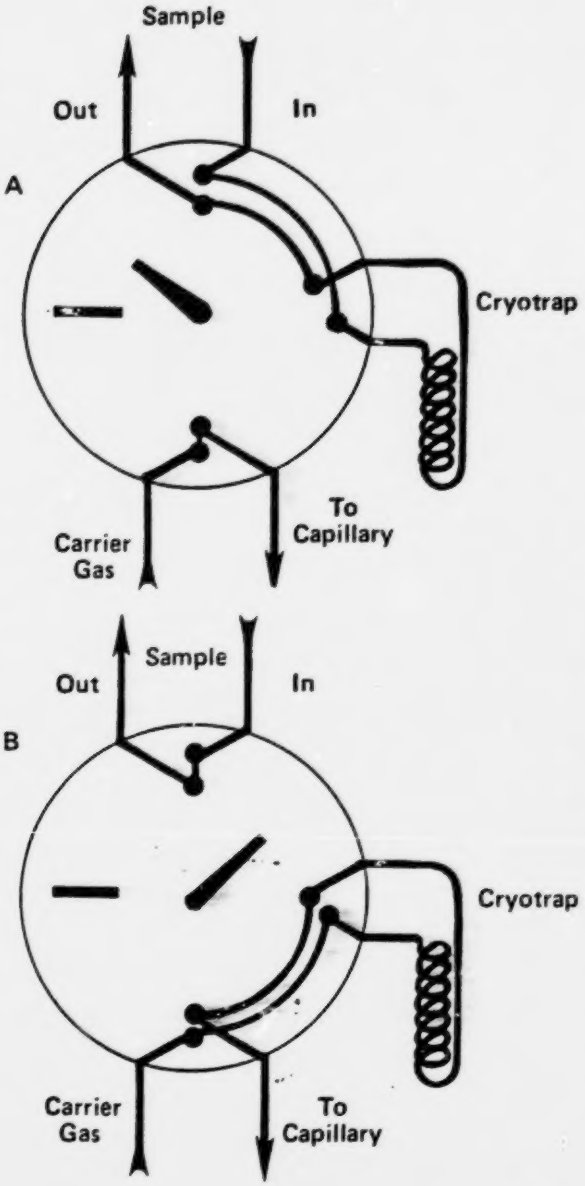

Sample
Out
In
A
Cryotrap
Carrier Gas
To Capillary
Sample
Out
In
B
Cryotrap
Carrier Gas
To Capillary

Figure A-5. Valco® valve flow pattern for positions A and B.

ASSEMBLY OF TEMPERATURE CONTROLLER MODULES

Two temperature control modules, each with three controlling channels, are needed, one for the purge and trap system and one for the injection port and cryofocussing devices. Wattlow Series 100 temperature controllers with Type J thermocouples are used for temperature control. Table A-1 provides a parts listing for the two sets of temperature controllers. Each temperature controller set is assembled for inclusion in a bud box. Figure A-6 shows a schematic of the control and readout circuits. Figure A-7 depicts the front panels of the two temperature control modules used for controlling the various heating elements on the purge and trap and injection port systems. As the front panels indicates, there are three channels per temperature control module with individual toggle switches for on/off of each channel as well as overall power. A six-position non-shorting rotary switch is used to monitor the temperatures of the various components. The temperature is read on a pyrometer (Figure A-7).

Temperature control module No. 1 is employed for controlling the Valco valve (8), Tenax trap (4), and sample lines (5,6,20,21 and 22) on the purge and trap system (Figure A-7). Temperature control module No. 2 is used to control the temperatures on the injection port block (1), cryofocussing system (2), and, when executing the NEWS protocol, the heating collar (8) on the purge and trap vessel. The six temperature control channels have separate thermocouples for heat control and temperature readout. In Figure A-6, the thermocouples found in control module No. 1 for the sample lines, Valco valve, and Tenax trap are shown. Control module No. 2 has thermocouples for the injection block, cryofocussing trap, and heating collar for the purge and trap vessel.

The temperature controller and sensor thermocouples and the pyrometers are calibrated against a standard source prior to their use on the purge and trap system.

FABRICATION OF PURGE AND TRAP SYSTEM

Figures A-7 and A-8 depict the front and rear views of the purge and trap system. A parts listing is given in Tables A-2 and A-4. A stand is fabricated that will hold an aluminum plate on a rack system anchored to a wooden

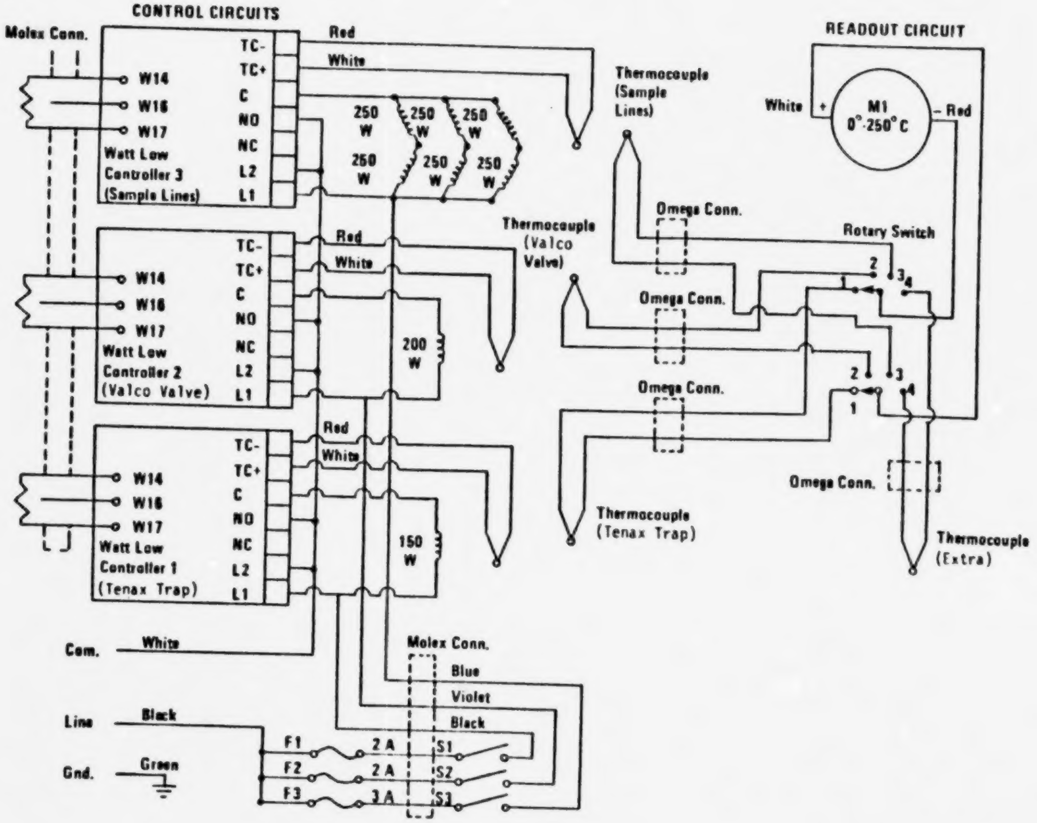

CONTROL CIRCUITS
Molex Conn.
W14
W16
W17
Watt Low Controller 3 (Sample Lines)
TC-
TC+
C
NO
NC
L2
L1
Red
White
250 W
250 W
250 W
250 W
250 W
250 W
Watt Low Controller 2 (Valco Valve)
200 W
Watt Low Controller 1 (Tenax Trap)
150 W
Com.
White
Line
Black
Gnd.
Green
F1
F2
F3
2 A
2 A
3 A
Molex Conn.
Blue
Violet
Black
S1
S2
S3
READOUT CIRCUIT
M1 0°-250°C
White
+
-
Red
Thermocouple (Sample Lines)
Thermocouple (Valco Valve)
Thermocouple (Tenax Trap)
Thermocouple (Extra)
Omega Conn.
Omega Conn.
Omega Conn.
Omega Conn.
Rotary Switch
1
2
3
4

Figure A-6. Schematic of control and readout circuits for temperature control module No. 1.

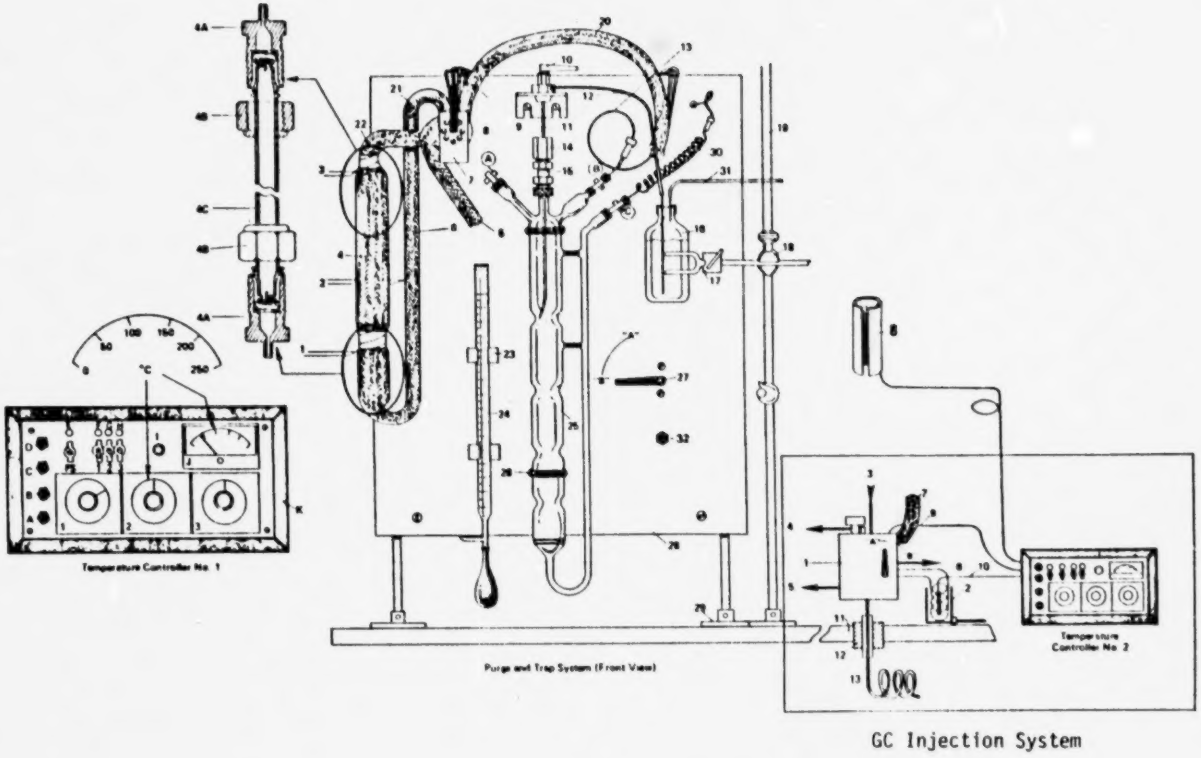

4A
4B
4C
4B
4A
0
50
100
150
200
250
°C
Temperature Controller No. 1
K
1
2
3
4
8
20
21
22
13
10
12
9
11
14
15
23
24
25
26
27
28
29
30
31
16
17
18
19
32
Purge and Trap System (Front View)
8
3
7
4
1
5
2
10
11
12
13
Temperature Controller No. 2
GC Injection System

Figure A-7. Purge and trap system with injection system.

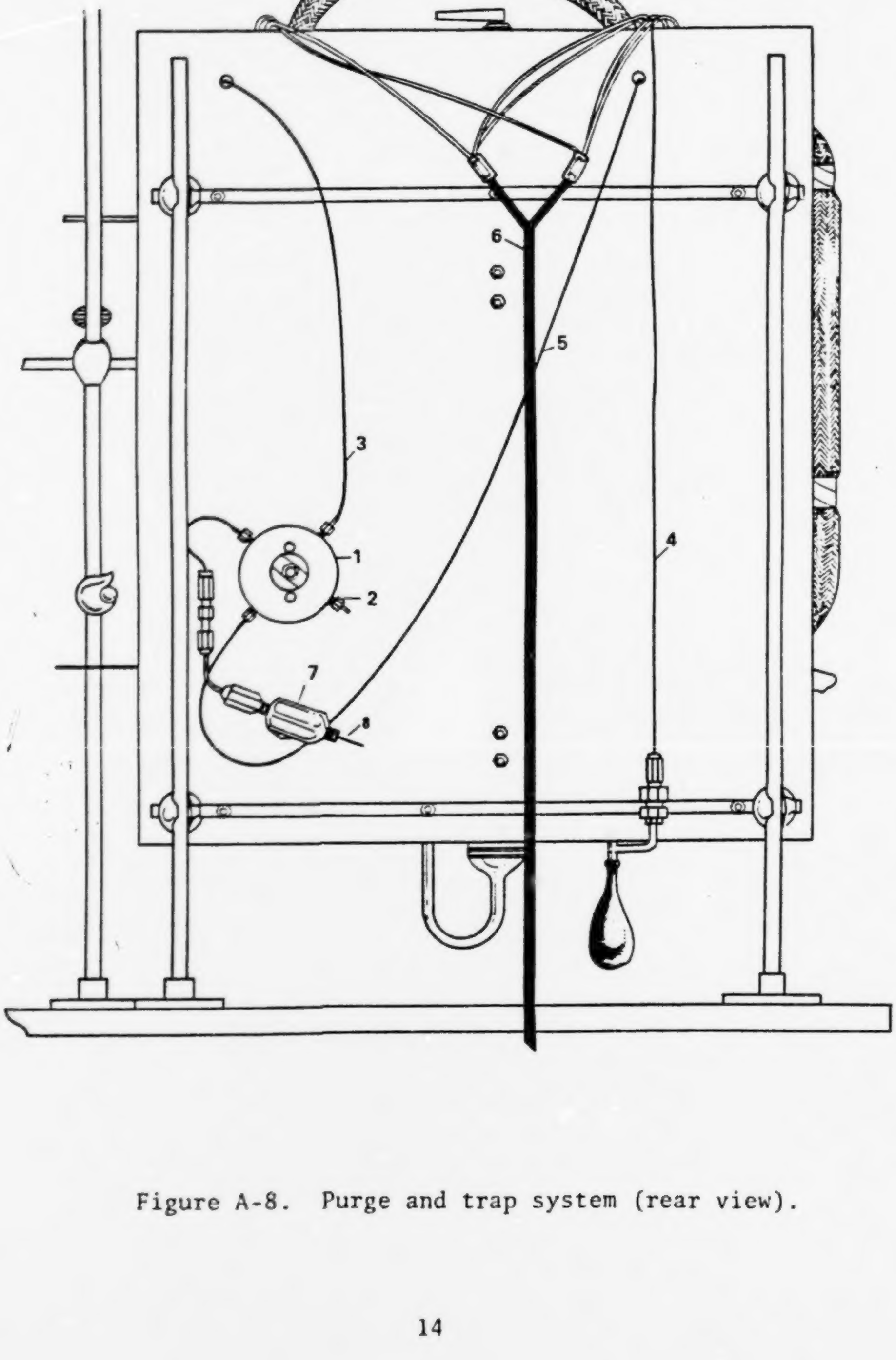


Figure A-8. Purge and trap system (rear view).

Table A-2. COMPONENT IDENTIFICATION - PURGE AND TRAP SYSTEM

Item #	Description
4	Sorbent trap (1.5 g Tenax GC; 35/60 mesh)
4A	3/8 in → 1/16 in stainless steel, fritted (10 μ) reducing union
4B	3/8 in stainless steel nut
4C	10 in × 3/8 in o.d. × 5/16 in i.d. stainless steel tubing
5	Heated/insulated nickel transfer line from 6-port valve to GC injection system (item 7 on right side of Fig. A-7), 1/16 in o.d. × 0.040 in i.d. × 30 in
6	Heated/insulated nickel transfer line from 6-port valve to sorbent trap, 1/16 in o.d. × 0.040 in i.d. × 14 in
7	Support for 6-port valve, Valco
8	Six-port valve, Valco C-6-T, 1/16 in zero dead volume fittings
9	Support bracket for sample valve, Tekmar 1400507000
10	Sample valve, Tekmar 14036
11	Sample introduction needle, Tekmar 14-0033-053
12	Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × ~20 in) with needle (18 gauge × 14 cm)
13	Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × 8 in) with Cheminert® connector (LDC) for connecting to item 20
14 15	Sampler union, Tekmar 14049
16	Sample container, 243 mL, glass, 24 mm septum cap
17	Three-finger clamp, Fisher 05-742
18	Clamp holder, Fisher 05-754
19	Aluminum rod, 1/2 in, Fisher 14-666
20	Heated/insulated nickel transfer line from purge flask connecting line (item 13) to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 14 in
21	Heated/insulated nickel transfer line from 6-port valve to sorbent trap, 1/16 in o.d. × 0.040 in i.d. × 20 in
22	Heated/insulated nickel transfer line from sorbent trap to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 5 in
23	Clamp
24	Soap bubble flowmeter

(continued)

Table A-2 (cont'd.)

Item #	Description
25	Purge flask (See Chapter 6, MAS protocols, for details): Approximate dimensions - 45 cm × 3.5 cm Purge gas inlet - 1/16 in o.d. Frit porosity - medium Material - borosilicate glass A: Microflex® valve, Kontes K-749100-21 B: Chromaflex® column valve, Kontes K-423600 C: Chromaflex® column valve, Kontes K-423600
26	Spring, 1-1/2 in
27	Dry purge valve, 4-port, Valco C-4-T, 1/16 in zero dead volume fittings
28	Aluminum panel, 16 in × 26 in × 1/8 in
29	Flexframe foot plate, Fisher 14-666-25
30	Purge gas line, Teflon tubing (1/16 in o.d. × ~0.040 in i.d. × ~20 in) with Cheminert® fitting (LDC)
31	Teflon tubing (1/16 in o.d. × ~0.040 in i.d.) with stainless steel needle (18 gauge × 2.5 cm)
32	Purge gas flow metering valve, Nupro SS-2SG, 1/8 in fittings
	Unspecified Equipment
1	Rope heaters - Hotwatt, Inc., 250 watt, 120V, 60 in
2	Insulation - glass wool sleeve 1/2 in × 1/16 in thick
3	Glass fiber tape - Scotch 27®
4	Nickel tubing (surrounding 1/16 in Ni transfer lines) 1/8 in o.d. × 0.085 in i.d. This sleeve is used to distribute heat more evenly from heating rope to 1/16 in transfer line.
	Vendors
1	Valco Instruments Co., Box 19032, Houston, TX 77024
2	Tekmar Co., P. O. Box 37202, Cincinnati, OH 45222
3	Fisher Scientific Co., various locations
4	Kontes Glass, P. O. Box 739, Vineland, NJ 08360
5	Watlow Winona, Inc., 1265 E. Sanborn St., Winona, MN 55987
6	Hotwatt, Inc., 128 Maple St., Danvers, MA
7	Laboratory Data Control, P. O. Box 10235, Riviera Beach, FL 33404

base. The dimensions of the aluminum are 1/8 in × 16 in × 26 in. It is secured to the aluminum rack stand as indicated in Figure A-8. Holes are drilled through the aluminum plate and on the two crossbars of the aluminum rack and the holes are counter sunk on the plate for bolting the plate in place. All the components then are assembled as indicated in Figure A-7. The relationship of the purge and trap system (Figure A-7) with respect to the injection port system is also indicated. The purge and trap stand should be conveniently located near the injection port system, which is mounted on the gas chromatograph. The Ni transfer line (5, Figure A-7) from the Valco valve (8) of the purge and trap system to the injection port system (right side of Fig. A-7, item 7) is generally 2-1/2 to 3 feet in length; its length is not critical since the sample will be focussed prior to injection onto the GC capillary. Table A-3 identifies the components of the injection system.

The parts listing for the rear view of the purge and trap system is given in Table A-4. For the proper assembly of the six-port and four-port valves, it is important to consult the flow diagrams which are provided with the valves by the manufacturer to insure that the gas flow is properly directed with each rotated position of the valve. Figure A-9 shows the flow pattern during the wet and dry purge steps through the purge and trap system. During purging of a water sample, the purge gas passes through the purge vessel, the six-port Valco® valve, Tenax GC® trap six- port valve and to the bubble meter (Valco valve in position A). During the "dry" purge step, the K-423600 valve (B, Fig. A-7) is closed and the gas is directed to the 1/16 in Swagelock® Tee Union, passing through six-port valve, Tenax GC® trap and to the bubble meter (Valco valve in position A). In either case the GC carrier gas passes through the six-port valve and to the injection port system. During thermal desorption of the Tenax GC® trap, the six-port valve is rotated to position B and the GC carrier gas is directed through the Tenax trap in the reverse direction and then to the injection port system.

Figure A-10 depicts the dimensions of the Tenax trap.

Table A-3. COMPONENT IDENTIFICATION - INJECTION SYSTEM

Item #	Description
1	Heating block, containing 6-port valve (Valco C-6-T)
2	Nickel capillary cryogenic trap
3	Gas chromatograph carrier gas inlet to injector
4	Septum sweep (outlet), closed during operations.
5	Splitter exit (closed)
6	Vent
7	heater/insulated transfer line from 6-port valve on purge and trap system to injector body, 1/16 in o.d. × 0.040 in i.d. × 30 in (other end of item No. 5, Table A-2)
8	Purge flask heater, 3/4 in diameter × 8 in, Watlow 01808081
9	Electrical connection to injector body heater
10	Electrical connection to cryogenic trap heater
11	Gas chromatograph bulkhead
12	Gas chromatograph injection port
13	Capillary GC column

Table A-4. COMPONENT IDENTIFICATION - PURGE AND TRAP SYSTEM (REAR VIEW)

Item #	Description
1	Dry purge valve, 4-port, Valco C-4-T
2	Capped port
3	Purge gas line to purge flask, 1/16 in o.d. × 0.040 in i.d. × 12 in (connected to line 30, see Fig. A-7)
4	Vent from 6-port valve for monitoring purge gas flow, 1/16 in o.d. × 0.040 in i.d. × 20 in
5	Dry purge line to 6-port valve, 1/16 in o.d. × 0.040 in i.d. × 24 in
6	Heater cable connections to purge and trap temperature controller
7	Purge gas flow metering valve, Nupro SS-2SG
8	Gas line from helium cylinder, 1/8 in copper

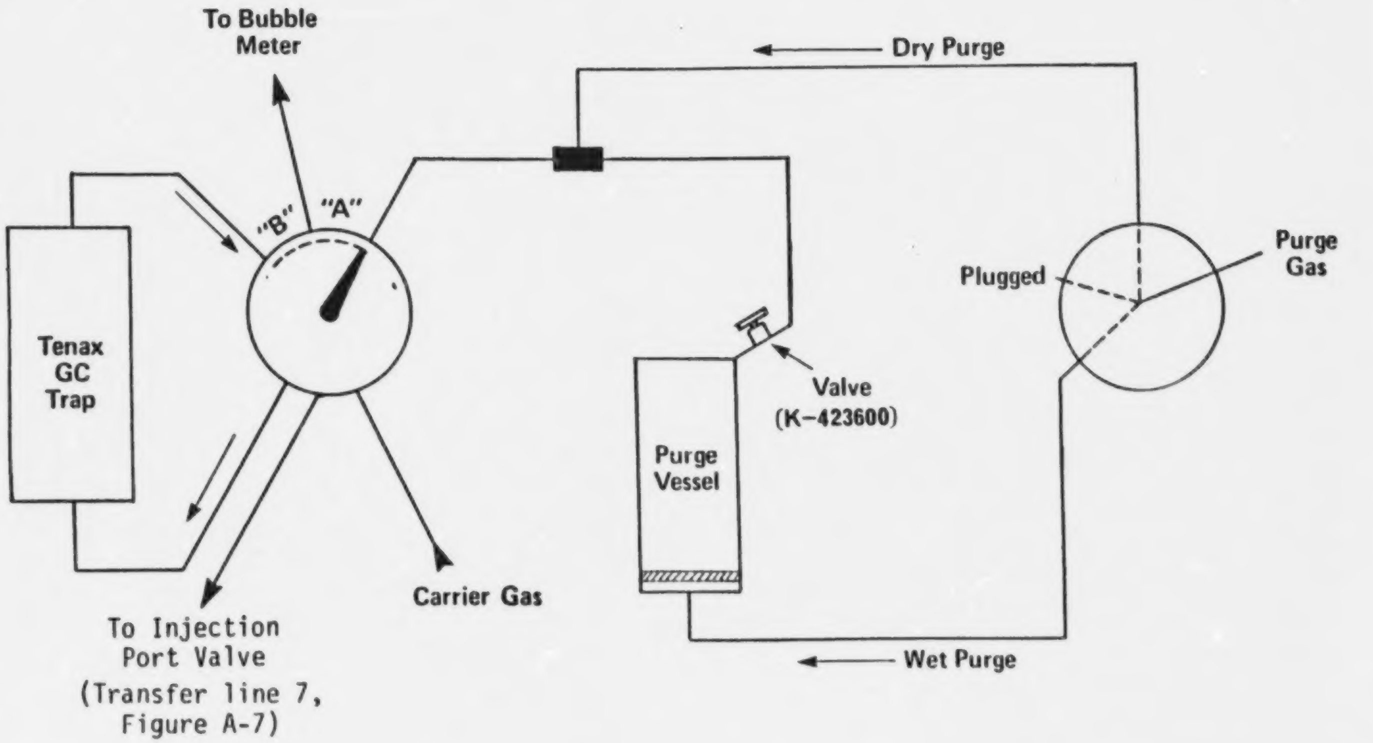

To Bubble Meter
"B"
"A"
Tenax GC Trap
To Injection Port Valve (Transfer line 7, Figure A-7)
Carrier Gas
Dry Purge
Purge Vessel
Valve (K-423600)
Plugged
Purge Gas
Wet Purge

Figure A- 9. Flow diagram of purge and trap system.

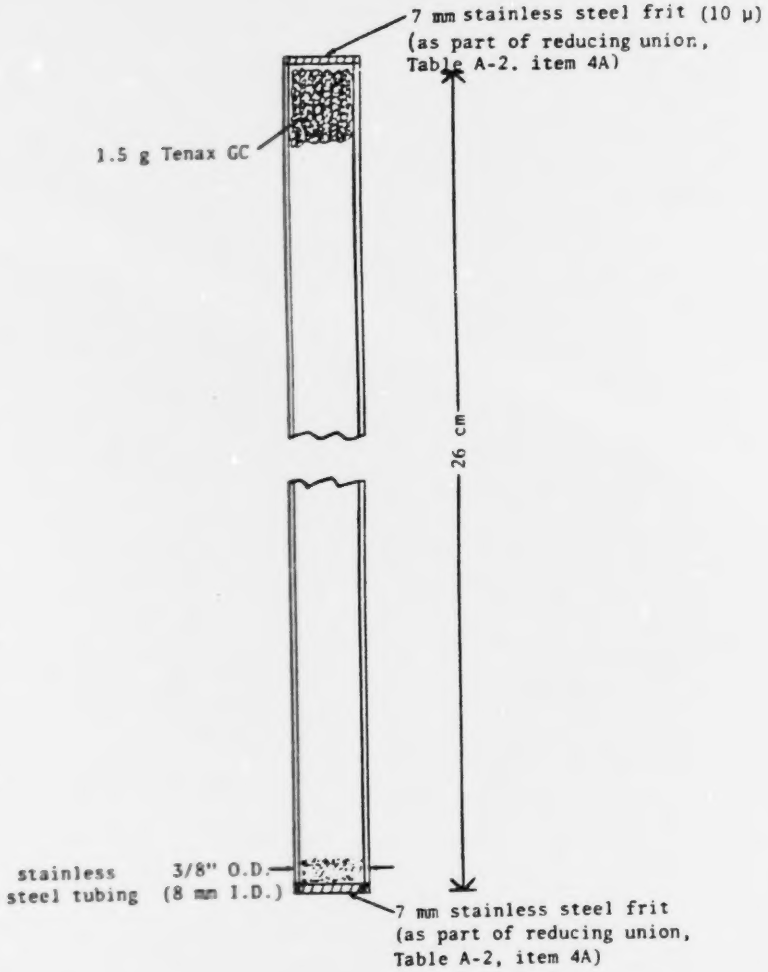

7 mm stainless steel frit (10 μ)
(as part of reducing union,
Table A-2. item 4A)
1.5 g Tenax GC
26 cm
stainless
steel tubing
3/8" O.D.
(8 mm I.D.)
7 mm stainless steel frit
(as part of reducing union,
Table A-2, item 4A)

Figure A-10. Tenax trap for purge and trap system (Fig. A-7).

ASSEMBLY OF SAMPLE TRANSFER SYSTEM (VO ANALYSIS PROTOCOL ONLY)

Figure A-11 depicts a schematic of the volatile organic sample transfer system. This is an expansion of a portion of Figure A-7 which shows the relative position of the sample transfer system to the purge and trap vessel. A two-way valve (G) is employed to direct the "on/off" pressurization of the water sample container. Sixteenth inch Teflon tubing is used to connect the two-way valve (G) to a stainless steel needle (F) with its hub removed (18 gauge × 2.5 cm in length). The water sample is delivered into the purge and trap vessel using a stainless steel needle (D, Fig. A-11), also with its hub removed (18 gauge × 14 cm in length), which is attached to a 1/16" Teflon tubing (E) and the three-way sample valve [Fig. A-7 (10)]. The long and short stainless steel needles are inserted respectively through the Teflon faced septum (H) just prior to transfer of the sample.

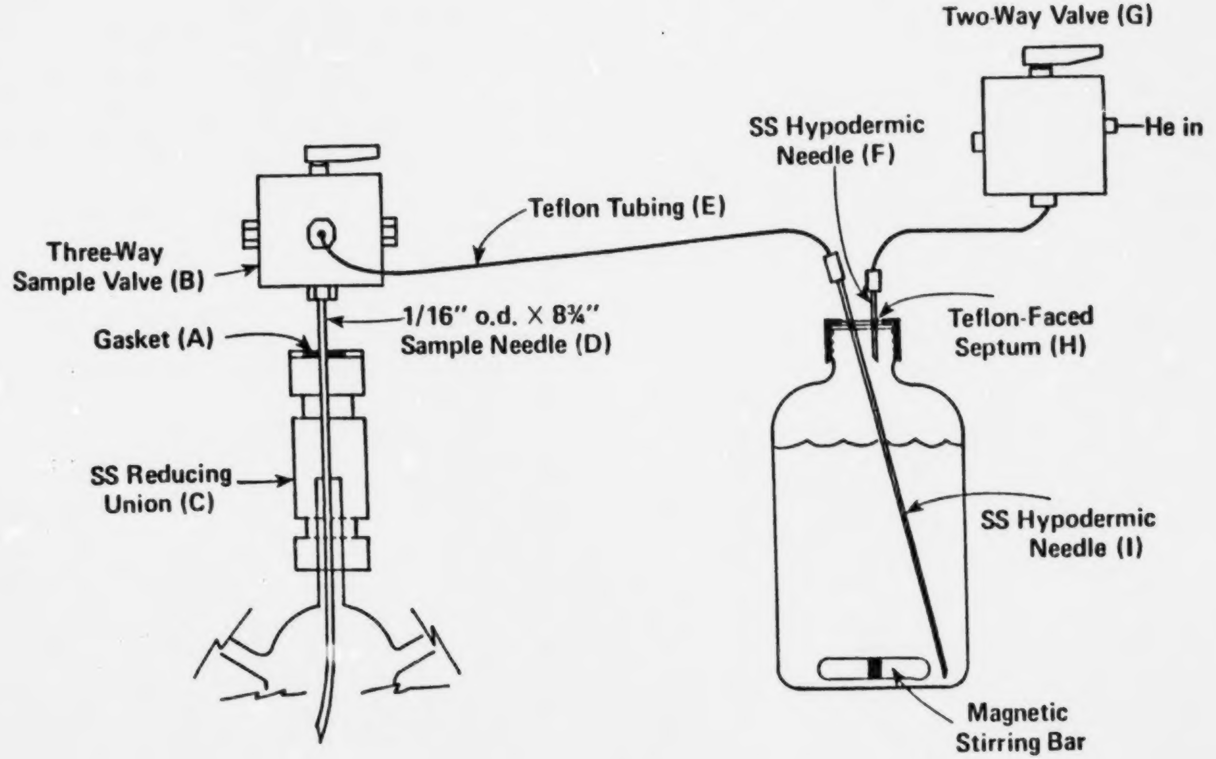

Two-Way Valve (G)
He in
SS Hypodermic Needle (F)
Teflon Tubing (E)
Three-Way Sample Valve (B)
1/16" o.d. × 8¾" Sample Needle (D)
Gasket (A)
Teflon-Faced Septum (H)
SS Reducing Union (C)
SS Hypodermic Needle (I)
Magnetic Stirring Bar

Figure A-11. Schematic of VO sample transfer system.

APPENDIX B

RMR AND RECOVERY DATA FILE FOR INTERNAL AND EXTERNAL STANDARDS AND ANALYTES IN MASQUANT

INTRODUCTION

This Appendix is basically a computer hard copy of recovery and relative molar response (RMR) factors of the Master Analytical Scheme's internal standards and its approximately 280 model compounds. These data are part of the computer files for MASQUANT, a program for calculation of concentrations of analytes detected during implementation of the MAS. The user should refer to Chapter 1 (Section 1.2.7) and Chapter 13 (Section 13.4.2.2) of "Part 1: Protocols" for a discussion of the general approach towards quantitation, whether conducted manually or using MASQUANT.

GENERAL DESCRIPTION OF MASQUANT

MASQUANT has been written to carry out some of the basic calculations used to process data obtained using the Master Analytical Scheme. MASQUANT consists of approximately 2,000 lines of source code written in ANSI subset Fortran 77, which should make it operable on any computer capable of handling this language.

The program consists of a main routine and sixteen subroutines, which will be described in greater detail in Appendix C. The program is written to run interactively, with a continuing dialogue between the user and the computer. After all of the data are processed, a report giving the calculated concentration of each identified component is generated.

In order to use MASQUANT, three files need to be accessed from an external disk or tape. The files are organized in a sequential fashion, and are read or written to in this same manner. These files are 1) a file which contains calculated correction factors for RMRs which can be applied to the library file, if desired; 2) a standard file consisting of internal and external standards, along with associated data including recovery factors and response factors; and 3) a file, written in the identical format as file 2, consisting of data for "unknown" analytes. The compounds and standards are organized into 13 clases, consistent with the MAS Protocols. Detailed formats for the three files are given in Appendix C.

USE OF TABLES

The following table lists the 13 classes of MAS compounds and standards for use with MASQUANT, with page numbers of corresponding data tables. Each table is in three parts: 1) a table of internal and external standards and their identification numbers; 2) a tabulated matrix of standard ion RMRs, which requires more than one page for Classes 3-8; and 3) a table of MASQUANT computer output of recoveries and RMRs of analytes (MAS model compounds), which often requires several pages for each class.

Table	Class No.	Class	Page
B-1	1	RMRs and Recoveries for VO Compounds	27
B-2	2	RMRs and Recoveries for NEWS Compounds	35
B-3	3	RMRs and Recoveries WABN Compounds (BLLE, pH 8.0/No Fractionation)	40
B-4	4	RMRs and Recoveries for WABN Compounds (BLLE, pH 8.0/Fraction No. 1)	61
B-5	5	RMRs and Recoveries for WABN Compounds (BLLE, pH 8.0/Fraction Nos. 2 & 3)	82
B-6	6	RMRs and Recoveries for WABN Compounds (BLLE, pH 8.0/Fraction No. 3)	103
B-7	7	RMRs and Recoveries for WABN Compounds (FU, pH 8.0)	124
B-8	8	RMRs and Recoveries for WABN Compounds (Accumulator Column, pH 8.0)	145
B-9	9	RMRs and Recoveries for ESSA Compounds	166
B-10	10	RMRs and Recoveries for VOSA Compounds	171
B-11	11	RMRs and Recoveries for NOVA Compounds	175
B-12	12	RMRs and Recoveries for SAM-PT Compounds	178
B-13	13	RMRs and Recoveries for SAM-S Compounds	181

Following are explanations of the MASQUANT computer output hard copy.

For each compound (analyte) listing, data is arranged as follows:

First line: Compound # Recovery Compound name and CAS number

Second and third lines: Analyte ion (m/z) Analyte RMRs vs. standard ions

Standard ions are listed at the top of each page under the standard number. There are usually two ions listed for each standard (and two for each analyte). See the first table in each class for identification of standards by number.

Definitions/Explanations:

Compound #: compound (analyte) number assigned in MASQUANT

Analyte ion: ion (m/z) of analyte for which an RMR has been determined. There are usually two for each compound.

Recovery: recovery determined for the analyte using the prescribed protocol; e.g., 1.00 = 100%, 0.97 = 97%. Compounds whose recovery have not been determined using the prescribed protocol are assigned a numerical value of 0.01.

RMR (relative molar response): space is allocated for two RMR values for each analyte ion measured against each standard. If a standard contains only one ion, a dash (-) is placed at the heading of the second column and no values are listed in that column. A RMR of *** is greater than 9.99; a RMR of 0.00 is less than 0.01. All RMRs were determined using a Finnigan 4021 GC/MS with an Incos Data System.

NOTE: Classes 3-8 use more than 5 standards; there is room for only 5 per page, so there are 2 pages of data for each analyte for these classes.

Table B-1. RMRs AND RECOVERIES FOR VO COMPOUNDS

Class No. 1

Standard ID No.	Standard Name
1	perfluorotoluene (external)
51	d_5-Bromoethane (internal)
52	2,4,6-d_3-Anisole (internal)
53	d_5-Chlorobenzene (internal)
54	d_8-Naphthalene (internal)

MATRIX OF STANDARD ION RMRs

			Standard									
			Perfluorotoluene		2,3,6-d_3-Anisole		d_5-Chlorobenzene		d_{10}-Diethyl ether		d_5-Bromoethane	
Standard	Ion	Recovery	m/z 186	m/z 236	m/z 81	m/z 111	m/z 82	m/z 117	m/z 50	m/z 66	m/z 113	m/z 115
perfluorotoluene	186	NA	-	.93(3)[a]	1.30(27)	.70(27)	1.13(6)	.55(14)	3.11(270	1.46(28)	1.57(21)	1.61(22)
	236	NA	1.08(3)	-	1.41(25)	.75(25)	1.19(13)	.58(11)	3.30(24)	1.54(25)	1.69(19)	1.73(20)
2,4,6-d_3-anisole	81	0.57	.82(29)	.76(28)	-	.54(1)	.92(17)	.45(18)	2.87(45)	1.32(44)	1.55(34)	1.60(36)
	111	0.57	1.53(30)	1.42(27)	1.87(1)	-	1.71(17)	.84(17)	5.35(45)	2.45(44)	2.88(34)	2.97(35)
d_5-chlorobenzene	82	1.20	.91(19)	.85(16)	1.11(16)	.60(17)	-	.49(2)	3.07(24)	1.43(23)	1.65(18)	1.70(18)
	117	1.20	1.87(17)	1.75(14)	2.25(18)	1.23(17)	2.05(2)	-	6.31(24)	2.92(22)	3.38(18)	3.49(19)
d_{10}-diethyl ether	50	NA	.34(22)	.31(21)	.41(45)	.22(45)	.35(27)	.17(25)	-	.46(2)	.57(21)	.58(22)
	66	NA	.72(24)	.67(22)	.88(44)	.48(44)	.75(26)	.37(25)	2.16(2)	-	1.23(20)	1.27(20)
d_5-bromoethane	113	0.85	.66(21)	.61(19)	.71(30)	.38(31)	.63(16)	.31(17)	1.82(19)	.83(18)	-	1.03(1)
	115	0.85	.64(22)	.59(19)	.69(30)	.37(31)	.61(17)	.30(17)	1.76(20)	.81(19)	.97(1)	-

[a] (CV)

Note: This matrix was generated before final internal standards were selected. The correct standards are listed on the first part of Table B-1 (preceeding page). The matrix as shown here includes d_{10}-diethyl ether, but omits d_8-naphthalene. However, on the RMR and recovery tables on pp. 29-34, values for standards 1, 52, 53, and 54 are given; i.e., naphthalene is included but bromoethane and diethyl ether are not. (There are a few exceptions where bromoethane is used, but naphthalene is not.)

```
          Internal/External Standard File for Cmpd Class # 1

Cmpd#   Recovery   Compound Name
         Std # 1      Std #51      Std #52       Std #53      Std #54
Mass    186   236    113   115     81   111     82   117    136    -


  105     1.25      TOLUENE 108883
  91   2.05  1.89                2.25   1.21   2.13  1.04   0.32
  92   1.32  1.21                1.44   0.78   1.37  0.67   0.20

  106     0.01      O-XYLENE 95476
  91   2.00  1.87                2.45   1.32   2.29  1.09   0.34
 106   1.10  1.03                1.35   0.73   1.25  0.60   0.19

  107     0.98      P-XYLENE 106423
  91   1.84  1.62                2.81   1.39   2.39  1.07   0.33
 106   1.07  0.95                1.56   0.86   1.48  0.65   0.20

  108     0.96      ETHYLBENZENE 100414
  93   3.18  2.12                3.47   1.88   3.30  1.60   0.49
 106   1.11  1.02                1.21   0.65   1.15  0.55   0.17

  109     0.01      2-METHYLSTYRENE 611154
 117   0.78  0.74                0.93   0.50   0.88  0.42   0.13
 118   0.98  0.93                1.18   0.63   1.11  0.53   0.16

  110     0.77      1,3,5-TRIMETHYLBENZENE 108678
 105   4.02  3.80                4.80   2.58   4.54  2.16   0.65
 120   2.37  2.24                2.83   1.52   2.68  1.27   0.38

  111     0.94      1,2,4-TRIMETHYLBENZENE 95636
 105   2.23  1.95                3.20   1.73   2.98  1.32   0.38
 120   1.26  1.11                1.85   1.03   1.79  0.78   0.21

  112     0.01      ISOPROPYLBENZENE 98828
 105   2.73  2.27                3.11   1.68   2.60  1.23   0.49
 120   0.82  0.69                0.95   0.51   0.78  0.37   0.15

  113     0.01      O-ETHYLTOLUENE 611143
 105   3.38  3.11                3.70   2.00   3.52  1.71   0.52
 120   1.14  1.05                1.24   0.67   1.18  0.58   0.18

  114     0.01      P-ETHYLTOLUENE 622968
 105   3.20  2.99                3.92   2.12   3.66  1.75   0.54
 120   1.05  0.98                1.28   0.69   1.19  0.57   0.18

  115     1.13      SEC-BUTYLBENZENE 135988
 105   3.69  3.09                4.30   2.32   3.54  1.68   0.67
 134   0.89  0.75                1.04   0.56   0.86  0.41   0.16

  116     0.81      P-DIETHYLBENZENE 105055
  91   0.61  0.56                0.67   0.36   0.63  0.31   0.09
 119   2.37  2.18                2.59   1.40   2.47  1.20   0.37

  117     1.00      4-METHYLISOPROPYLBENZENE 99876
 119   3.35  3.18                4.00   2.15   3.79  1.80   0.54
 134   0.95  0.90                1.14   0.61   1.08  0.51   0.15
```

```
        Internal/External Standard File for Cmpd Class # 1

Cmpd#    Recovery   Compound Name
          Std # 1     Std #51      Std #52      Std #53      Std #54
Mass     186   236   113   115    81   111     82   117     136     -


 118       0.74     NAPHTHALENE 91203
 128    4.46  3.93                6.67  3.56   5.71  2.73    0.78

 119       0.59     DIPHENYLMETHANE 101815
 167    2.98  2.49                3.45  1.86   2.85  1.35    0.54
 168    3.18  2.62                3.63  1.96   2.99  1.42    0.57

 120       1.13     TERT-BUTYLBENZENE 98066
 119    2.64  2.47                3.24  1.75   3.02  1.44    0.45
 134    0.67  0.63                0.83  0.45   0.77  0.37    0.11

 121       1.16     FLUOROBENZENE 462066
  70    0.30  0.25                0.35  0.19   0.29  0.14    0.05
  96    1.49  1.24                1.73  0.93   1.42  0.68    0.27

 122       0.91     CHLOROBENZENE 108907
  77    0.83  0.73                1.25  0.62   1.03  0.46    0.15
 112    1.65  1.46                2.32  1.33   2.32  0.98    0.29

 123       1.23     BROMOBENZENE 108861
  77    1.90  1.59                2.21  1.19   1.82  0.87    0.35
 156    1.27  1.06                1.53  0.82   1.22  0.58    0.23

 124       0.01     BENZYLCHLORIDE 100447
  91    1.83  1.73   3.31  3.42   2.83  1.52   2.21  1.06
 126    0.46  0.44   0.84  0.86   0.71  0.38   0.56  0.27

 125       1.04     P-BROMOTOLUENE 106387
  91    1.99  1.89                2.39  1.28   2.25  1.07    0.32
 170    1.00  0.95                1.20  0.64   1.13  0.54    0.16

 126       1.06     IODOTOLUENE(P) 624317
  91    2.18  1.82                2.62  1.41   2.15  1.02    0.39
 218    2.82  2.36                3.39  1.83   2.70  1.28    0.51

 127       1.16     1,2-DICHLOROBENZENE 541731
 111    0.85  0.71                0.99  0.53   0.82  0.39    0.15
 146    2.36  1.97                2.74  1.48   2.26  1.07    0.43

 128       1.03     1,3-DICHLOROBENZENE 95501
 111    0.78  0.73                0.93  0.50   0.88  0.42    0.13
 146    2.24  2.11                2.66  1.43   2.52  1.26    0.36

 129       0.83     1,4-DICHLOROBENZENE 106467
 111    0.92  0.84                1.00  0.54   0.95  0.47    0.14
 146    2.73  2.51                2.99  1.61   2.84  1.28    0.42

 130       0.92     2-BROMOCHLOROBENZENE 694804
 196    1.53  1.40                1.67  0.90   1.59  0.78    0.24
 192    2.03  1.86                2.22  1.20   2.11  1.03    0.31
```

```
            Internal/External Standard File for Cmpd Class # 1

Cmpd#    Recovery   Compound Name
           Std # 1     Std #51        Std #52       Std #53       Std #54
Mass     186   236    113   115     81    111     82   117     136      -


  131      1.06     4-BROMOCHLOROBENZENE 106398
 190    1.34  1.27                  1.60  0.86    1.52  0.72    0.22
 192    1.81  1.68                  2.12  1.14    2.01  0.96    0.29

  132      1.01     1,2,4-TRICHLOROBENZENE 120821
 180    1.83  1.62                  2.72  1.46    2.32  1.11    0.33
 182    1.80  1.59                  2.68  1.44    2.28  1.09    0.32

  133      0.70     A,A,A,TRICHLOROTOLUENE 98077
 159    1.63  1.52                  1.85  1.03    2.09  1.03    0.27
 161    1.10  1.02                  1.24  0.69    1.41  0.70    0.18

  134      0.01     3-CHLOROBENZONITRILE
 102    1.13  0.97                  1.35  0.73    1.11  0.53    0.21
 137    4.22  3.63                  5.03  1.41    4.15  1.97    0.78

  135      0.68     ANISOLE 100663
  78    0.71  0.66                  0.87  0.47    0.81  0.39    0.12
 108    1.27  1.20                  1.57  0.85    1.46  0.70    0.22

  136      0.47     BIPHENYL ETHER 101848
  77    1.18  1.08                  1.28  0.69    1.22  0.60    0.18
 170    3.57  3.28                  3.90  2.11    3.70  1.81    0.55

  137      0.01     BENZYL ETHER 103504
  91    4.37  4.13                  5.20  2.80    1.52  2.35    0.70
  92    5.60  5.30                  6.67  3.58    2.01  3.01    0.90

  138      0.67     PROPYLENE OXIDE 75569
  29    0.52  0.47    0.69  0.70    0.56  0.30    0.49  0.25
  58    0.27  0.24    0.35  0.36    0.28  0.15    0.25  0.12

  139      1.15     DIETHYL ETHER 60297
  31    1.89  1.72    2.50  2.55    2.00  1.07    1.75  0.88
  59    0.62  0.56    0.82  0.83    0.65  0.35    0.57  0.28

  140      0.80     2-METHYLFURAN 534225
  53    0.48  0.45    0.86  0.88    0.74  1.57    0.58  0.28
  82    0.77  0.73    1.39  1.43    1.20  0.22    0.93  0.45

  141      0.98     ALLYL ETHER 557404
  41    1.88  1.77    3.39  3.50    2.92  0.40    2.28  1.09
  69    0.27  0.25    0.48  0.50    0.42  0.64    0.33  0.15

  142      0.70     HEXYL ETHER 112583
  43    4.29  3.97                  4.83  2.68    5.42  2.68    0.71
  85    3.53  3.26                  3.97  2.20    4.47  2.21    0.58

  143      1.00     CARBON DISULFIDE 75150
  76    2.26  2.06    3.00  3.06    2.37  1.27    2.07  1.04
```

```
            Internal/External Standard File for Cmpd Class # 1

Cmpd#     Recovery    Compound Name
           Std # 1      Std #51        Std #52       Std #53       Std #54
Mass      186   236    113   115      81    111     82    117     136    -


 144        1.20      THIOPHENE 110021
  58     0.49  0.47                  0.58  0.31    0.55  0.26    0.08
  84     0.97  0.92                  1.16  0.62    1.10  0.52    0.16

 145        1.13      CYCLOPENTANE 287923
  42     1.84  1.68    2.44  2.49    1.91  1.02    1.68  0.84
  70     0.47  0.43    0.63  0.64    0.50  0.27    0.44  0.22

 146        0.85      CYCLOHEXANE 110827
  56     1.34  1.26    2.41  2.49    2.08  1.12    1.62  0.77
  84     0.99  0.93    1.78  1.84    1.54  0.83    1.20  0.57

 147        1.05      HEXANE 110543
  43     0.89  0.83                  1.09  0.59    1.02  0.48    0.15
  47     0.69  0.65                  0.85  0.46    0.79  0.38    0.12

 148        1.20      HEPTANE 142825
  57     0.61  0.56                  0.67  0.36    0.63  0.31    0.09
  71     0.63  0.57                  0.68  0.37    0.64  0.31    0.10

 149        0.01      1-OCTENE 111660
  41     0.92  0.76                  1.06  0.57    0.88  0.42    0.17
  55     0.73  0.61                  0.85  0.46    0.70  0.33    0.13

 150        1.03      OCTANE 111659
  43     1.54  1.36                  2.13  1.22    1.78  0.94    0.27
  57     0.52  0.46                  0.71  0.41    0.60  0.32    0.09

 151        0.79      NONANE 111842
  43     2.27  2.13                  2.79  1.51    2.60  1.24    0.38
  57     1.69  1.58                  2.07  1.12    1.93  0.92    0.28

 152        0.96      DIPENTENE 5989275
  68     0.61  0.52                  0.95  0.47    0.76  0.33    0.11
 136     0.14  0.11                  0.22  0.12    0.19  0.08    0.02

 153        0.89      N-DECANE 629505
  57     2.76  2.56                  3.11  1.73    3.50  1.73    0.46
  71     1.07  0.98                  1.20  0.67    1.35  0.67    0.18

 154        0.50      N-UNDECANE 1120214
  43     2.55  2.41                  3.04  1.63    2.88  1.37    0.41
  57     2.70  2.56                  3.22  1.73    3.05  1.45    0.43

 155        0.67      N-DODECANE 112403
  43     2.90  2.42                  3.36  1.81    2.77  1.32    0.52
  57     2.99  2.50                  3.46  1.87    2.86  1.36    0.54

 156        0.44      N-TRIDECANE 629505
  43     2.98  2.82                  3.56  1.91    3.37  1.60    0.48
  57     3.56  3.37                  4.24  2.28    4.02  1.91    0.57
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```
             Internal/External Standard File for Cmpd Class # 1

 Cmpd#    Recovery    Compound Name
           Std # 1      Std #51        Std #52        Std #53        Std #54
 Mass     186   236    113   115      81   111       82   117      136    -


   157      0.49      N-TETRADECANE 629594
    57   2.19  2.03                 2.47  1.37    2.78  1.37    0.36
    71   1.28  1.18                 1.44  0.80    1.62  0.80    0.21

   158      0.01      BROMOMETHANE 74839
    94   1.05  0.99   1.91  1.96    1.63  0.87    1.27  0.61
    96   0.99  0.93   1.79  1.84    1.52  0.82    1.19  0.57

   159      0.01      DICHLOROMETHANE 75092
    49   1.47  1.34   1.95  1.15    1.55  0.83    1.35  0.68
    84   0.85  0.77   1.12  0.73    0.89  0.47    0.78  0.39

   160      0.95      BROMOCHLOROMETHANE 74975
    49   0.95  0.90   1.71  1.76    1.47  0.79    1.15  0.55
   130   0.60  0.56   1.08  1.11    0.93  0.50    0.72  0.35

   161      0.78      CHLOROFORM 67663
    83   1.24  1.17   2.24  2.31    1.93  1.03    1.50  0.72
    85   0.81  0.77   1.47  1.51    1.26  0.68    0.99  0.47

   162      0.01      VINYL CHLORIDE 75014
    62   1.06  0.97   1.41  1.44    1.11  0.59    0.97  0.49
    64   0.33  0.30   0.44  0.45    0.34  0.18    0.30  0.15

   163      0.87      TRANS-1,2-DICHLOROETHYLENE 540590
    61   0.93  0.85   1.23  1.26    0.47  0.52    0.85  0.43
    96   0.65  0.59   0.86  0.88    0.68  0.36    0.59  0.30

   164      1.02      1,2-DICHLOROETHANE 107062
    62   0.52  0.48                 0.57  0.31    0.54  0.26    0.08
    98   0.12  0.11                 0.14  0.07    0.13  0.06    0.02

   165      0.77      1,2-DIBROMOETHANE 106934
   107   1.68  1.38                 1.91  1.03    1.58  0.75    0.30
   109   1.54  1.29                 1.79  0.79    1.48  0.70    0.28

   166      1.18      TRICHLOROETHYLENE 79016
    95   0.69  0.66                 0.83  0.45    0.79  0.38    0.11
   130   0.77  0.73                 0.92  0.49    0.87  0.42    0.12

   167      0.01      1,1,2-TRICHLOROETHANE 79005
    97   0.75  0.69                 0.91  0.49    0.87  0.41    0.13
    99   0.47  0.44                 0.57  0.31    0.54  0.26    0.08

   168      0.64      ALLYL CHLORIDE 107051
    39   0.78  0.71   1.03  1.05    0.83  0.44    0.72  0.36
    41   1.23  1.12   1.63  1.66    1.28  0.69    1.12  0.56

   169      0.77      TETRACHLOROETHYLENE 127184
   164   0.83  0.71                 1.27  0.72    1.17  0.50    0.15
   166   1.08  0.93                 1.65  0.94    1.54  0.66    0.19
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            Internal/External Standard File for Cmpd Class # 1

Cmpd#    Recovery    Compound Name
          Std # 1      Std #51      Std #52        Std #53        Std #54
Mass     186   236     113   115     81   111       82   117       136    -


  170       1.28     1,2-DICHLOROPROPANE 78875
   62    0.50  0.44                  0.62  0.33    0.51  0.24    0.10
   63    0.72  0.60                  0.85  0.46    0.70  0.33    0.13

  171       0.99     2-BROMO-1-CHLOROPROPANE 3017956
   41    0.40  0.37                  0.47  0.26    0.54  0.27    0.07
   77    0.50  0.46                  0.58  0.32    0.68  0.33    0.08

  172       0.90     1,2-DIBROMOPROPANE 78751
  121    1.28  1.18                  1.40  0.75    1.33  0.64    0.20
  123    1.22  1.12                  1.33  0.72    1.27  0.62    0.19

  173       1.17     2-BROMOBUTANE 78762
   41    0.86  0.79                  0.97  0.54    1.09  0.54    0.14
   57    1.50  1.40                  1.70  0.94    1.92  0.95    0.25

  174       0.01     1,4-DICHLOROBUTANE 110565
   55    1.62  1.35                  1.92  1.03    1.57  0.75    0.29
   90    0.32  0.27                  0.38  0.20    0.31  0.15    0.06

  175       1.03     1,4-DIBROMOBUTANE 110521
   55    1.57  1.47                  1.93  1.04    1.80  0.86    0.27
  135    0.98  0.92                  1.21  0.65    1.13  0.54    0.17

  176       0.01     1-BROMO-2-METHYLBUTANE 10422352
   43    1.21  1.14                  1.49  0.80    1.39  0.66    0.20
   71    0.56  0.53                  0.69  0.37    0.65  0.31    0.09

  177       1.28     1-CHLOROHEXANE 544105
   55    0.69  0.65                  0.85  0.46    0.79  0.38    0.12
   91    1.00  0.93                  1.22  0.66    1.14  0.54    0.17

  178       1.29     1-BROMOHEXANE 111251
   43    1.66  1.52                  1.81  0.98    1.73  0.84    0.26
  135    0.54  0.50                  0.59  0.32    0.56  0.27    0.08

  179       0.01     1-BROMODECANE 112298
  135    1.45  1.34                  1.63  0.91    1.84  0.91    0.24
  137    1.56  1.44                  1.76  0.98    2.06  1.02    0.26

  180       0.76     BENZENE 71432
   78    1.77  1.67   3.18  3.28     2.75  1.47    2.14  1.02    0.21
```

Table B-2. RMRs AND RECOVERIES FOR NEWS COMPOUNDS

Class No. 2

Standard ID No.	Standard Name
1	Perfluorotoluene (external)
55	d_9-t-Butanol (internal)
56	d_5-Nitrobenzene (internal)

MATRIX OF STANDARD ION RMRs

			Standard					
			Perfluorotoluene		d_9-t-Butanol		d_5-Nitrobenzene	
Standard	Ion	Recovery	m/z 186	m/z 236	m/z 46	m/z 65	m/z 82	m/z 128
Perfluorotoluene	186	NA	-	1.18 (3)[a]	1.52 (16)	1.07 (21)	0.58 (8)	1.54 ± .14 (9)
	236	NA	0.96 (16)	-	1.73 (16)	1.24 (16)	0.68 (0)	1.77 ± .17 (10)
d_9-t-Butanol	46	0.98	0.61 (11)	0.51 (7)	-	0.64 (18)	0.47 (11)	1.82 ± .27 (15)
	65	0.98	1.01 (19)	0.81 (11)	1.51 (20)	-	0.79 (20)	2.89 ± .51 (17)
d_5-Nitrobenzene	82	0.93	1.30 (6)	1.13 (10)	2.25 (2)	1.32 (19)	-	3.99 ± .04 (1)
	128	0.93	0.59 (6)	0.51 (10)	1.07 (6)	0.59 (20)	0.46 (8)	-

[a] Coefficient of variation for triplicate determinations are given in parenthesis.

```
            Internal/External Standard File for Cmpd Class # 2

Cmpd#     Recovery    Compound Name
            Std # 1       Std #55        Std #56
Mass      186   236      46     65       82    128


  103       1.08      1-PROPANOL 71238
  42      0.14  0.06    0.19  0.07     0.04   0.21
  60      0.06  0.02    0.07  0.05     0.03   0.09

  104       1.20      1-BUTANOL 71363
  41      0.46  0.20    0.64  0.24     0.17   0.55
  56      0.42  0.18    0.57  0.39     0.28   0.49

  105       1.13      1-PENTANOL 71410
  42      0.77  0.33    1.30  0.40     0.29   1.00
  70      0.24  0.10    0.34  0.23     0.16   0.35

  107       1.22      CYCLOHEXANOL 108930
  57      0.07  0.03    0.10  0.01     0.01   0.12
  67      0.03  0.01    0.03  0.02     0.01   0.08

  108       1.31      1-HEXANOL 111273
  56      1.14  0.48    1.56  0.58     0.43   1.70
  84      0.05  0.03    0.08  0.06     0.04   0.09

  109       1.06      1-HEPTANOL 111706
  41      1.36  0.58    1.86  0.72     0.52   2.02
  70      0.97  0.42    1.33  0.64     0.92   1.45

  110       1.00      1-OCTANOL 111875
  41      0.94  0.39    1.16  0.49     0.34   1.40
  69      0.39  0.17    0.48  0.43     0.29   0.58

  112       0.01      BUTOXYETHANOL 111762
  41      0.45  0.54    0.81  0.47     0.40   0.76
  57      0.02  0.02    0.03  0.02     0.02   0.03

  114       0.99      PROPIONALDEHYDE 123386
  57      0.09  0.09    0.16  0.09     0.07   0.16
  59      0.03  0.03    0.05  0.03     0.02   0.04

  115       0.72      BUTYRALDEHYDE(N) 123728
  72      0.15  0.14    0.26  0.15     0.11   0.53

  116       0.83      CROTONALDEHYDE 4170303
  41      0.57  0.56    1.03  0.58     0.44   0.97
  70      0.32  0.32    0.47  0.28     0.26   0.55

  117       0.81      VALERALDEHYDE 110623
  44      0.64  0.63    1.16  0.66     0.50   1.09
  58      0.19  0.18    0.33  0.15     0.23   0.31

  118       0.45      FURFURAL 98011
  95      0.30  0.32    0.54  0.27     0.23   0.50
  96      0.29  0.31    0.53  0.29     0.23   0.49
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          Internal/External Standard File for Cmpd Class # 2

   Cmpd#    Recovery    Compound Name
             Std # 1       Std #55       Std #56
   Mass     186   236     46     65     82   128


     119       0.45      METHYL FORMATE 107313
     60     0.17  0.17    0.31  0.17    0.13  0.29

     120       0.59      METHYL ACETATE 79209
     43     1.75  1.71    3.16  1.80    1.80  3.00
     74     0.24  0.23    0.43  0.29    0.19  0.41

     121       0.53      ETHYL ACETATE 141786
     43     2.47  2.41    4.29  2.52    1.90  4.20
     61     0.24  0.44    0.44  0.27    0.19  0.42

     122       0.65      ALLYL ACETATE 591877
     43     3.10  3.02    5.61  3.17    2.39  5.26

     123       0.59      PROPYL ACETATE 109604
     43     3.21  3.12    5.80  3.29    2.47  5.45
     61     0.68  0.66    1.22  0.83    0.53  1.14

     124       0.45      ETHYL BUTYRATE 105544
     43     1.16  1.13    2.10  0.91    0.77  1.98
     71     0.87  0.84    1.57  0.95    0.68  1.47

     125       0.53      N-BUTYL ACETATE 123864
     43     2.79  2.70    5.04  2.20    1.97  4.74
     56     0.79  0.77    1.42  0.70    0.62  1.34

     126       0.79      TETRAHYDROFURAN 109999
     42     1.23  1.25    2.21  1.30    0.98  2.06
     72     0.30  0.56    0.56  0.38    0.24  0.53

     127       0.36      DIOXANE 123911
     88     0.17  0.18    0.26  0.19    0.14  0.18
     58     0.14  0.15    0.31  0.17    0.11  0.22

     128       0.01      ACETONE 67641
     43     1.54  1.52    2.79  1.55    1.19  2.62
     58     0.56  0.55    1.01  0.66    0.44  0.95

     129       0.69      METHYL ETHYL KETONE 78933
     43     2.34  2.28    4.23  2.37    1.80  3.98
     72     0.36  0.35    0.64  0.43    0.27  0.60

     130       0.52      CYCLOPENTANONE 120923
     55     0.69  0.83    1.25  0.72    0.62  1.13
     84     0.24  0.30    0.44  0.26    0.22  0.48

     131       0.52      CYCLOHEXANONE 108941
     55     0.68  0.80    1.24  0.72    0.61  1.15
     98     0.20  0.28    0.48  0.23    0.20  3.49

     133       0.59      ACRYLONITRILE 107131
     53     1.06  0.38    1.15  0.56    0.40  1.33
     52     0.89  0.45    1.46  1.11    0.70  1.58
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          Internal/External Standard File for Cmpd Class # 2

Cmpd#    Recovery    Compound Name
          Std # 1       Std #55       Std #56
Mass     186   236      46    65      82   128


  134       0.95     PROPIONITRILE 107120
   54    1.28  0.51   1.72  0.68    0.45  1.93
   55    0.19  0.09   0.27  0.19    0.13  0.30

  135       0.57     ISOBUTYRONITRILE 78820
   42    2.64  1.12   3.63  1.39    1.00  3.95
   68    1.09  0.46   1.50  1.04    0.72  1.64

  136       0.91     BENZONITRILE 100470
  103    4.10  1.74   2.11  1.83    1.54  2.30
   76    1.54  0.65   5.63  3.86    2.75  6.14

  137       0.96     NITROMETHANE 75525
   61    0.52  0.25   0.64  0.31    0.22  0.69
   46    0.46  0.20   0.72  0.56    0.39  0.88

  138       0.93     NITROPROPANE 108032 OR 79469
   41    1.87  0.73   2.36  0.91    0.65  2.56
   43    1.54  0.65   2.12  1.67    1.02  2.28

  139       0.96     NITROBENZENE 98953
   77    2.66  1.13   3.65  1.40    1.00  3.97
  123    1.16  0.49   1.59  1.10    0.77  1.73
```

Table B-3. RMRs AND RECOVERIES FOR WABN COMPOUNDS (BLLE, pH 8.0/NO FRACTIONATION)

Class No. 3

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	0.85	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	0.58	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	0.58	1.03(a)	.60(0)	-	.18(6)	1.07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	0.71	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	0.79	.97(4)	.57(10)	.95(10)	.16(3)	-	1.60(1)	2.35(17)	1.70(16)
	128	0.79	.61(2)	.35(9)	.59(9)	.10(1)	.63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	84	0.80	.42(15)	.25(24)	.42(24)	.071 ~~.74~~(18)	.44(16)	.70(15)	-	.73(2)
	112	0.80	.58(15)	.35(22)	.58(23)	.098(18)	.61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	0.73	1.09(4)	.65(13)	1.07(14)	.18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	0.73	2.85(5)	1.67(13)	2.78(14)	.48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	0.75	1.52(2)	.90(7)	1.50(8)	.25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	0.75	.46(2)	.27(8)	.45(7)	~~.76~~(3) .076	.48(3)	.76(4)	1.11(18)	.81(17)
d_{12}-perylene	264	0.80	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	0.84	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	NA	1.10(4)	.65(7)	1.08(8)	.18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	NA	1.43(4)	.84(6)	1.39(7)	.24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(Continued)

			Standard							
			d_5-Propiophenone		d_5-Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-Iodotoluene	
Compound	Ion	Recovery	m/z 82	m/z 110	m/z 110	m/z 125	m/z 264	m/z 188	m/z 109	m/z 236
d_5-phenol	99	0.85	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-o-xylene	98	0.58	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	0.58	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	0.71	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	0.79	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	0.79	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	0.80	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	0.80	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	0.73	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	0.73	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	0.75	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	0.75	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	0.80	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	0.84	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

[a] (CV).

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          Internal/External Standard File for Cmpd Class # 3

Cmpd#   Recovery    Compound Name
          Std # 2     Std #54        Std #56       Std #57       Std #58
Mass     109   236    136    -        82   128      98   116       84   112


 110       0.01     P-NITROANILINE 100016
  65    0.44  0.35   0.08           0.52  0.83    0.27  0.46    1.30  0.97
 138    0.56  0.45   0.11           0.67  1.07    0.35  0.58    1.68  0.22

 111       0.80     2,4-DIMETHYLQUINOLINE 1198374
 156    0.41  0.32   0.08           0.47  0.75    0.26  0.43    0.95  0.68
 157    2.01  1.54   0.37           2.31  3.59    1.27  2.11    4.64  3.31

 112       0.01     1,8-DIAMINONAPHTHALENE 569415
 114    0.03  0.02   0.00           0.04  0.06    0.02  0.03    0.09  0.06
 141    0.05  0.04   0.01           0.06  0.01    0.03  0.05    0.14  0.11

 113       0.84     NICOTINE 54115
  84    1.17  0.90   0.22           1.35  2.09    0.74  1.23    2.70  1.92
 133    0.28  0.21   0.05           0.32  0.49    0.17  0.29    0.63  0.45

 114       0.79     CARBAZOLE 86748
 167    3.73  2.88   0.69           4.30  6.66    2.37  3.92    9.36  6.67

 115       0.91     2-AMINOBIPHENYL 90445
 168    6.79  5.11   1.20           7.65 12.18    4.61  6.67   19.13 14.17
 169   12.72  9.45   2.22          14.15 22.54    7.42 12.30   35.40 26.19

 116       0.76     DIPHENYLAMINE 122394
 168    1.48  1.14   0.27           1.71  2.65    0.94  1.56    3.43  2.45
 169    2.79  2.15   0.52           3.22  4.99    1.77  2.93    6.45  4.60

 117       0.01     DICYCLOHEXYLAMINE 101837
  56    0.33  0.37   0.06           0.39  0.63    0.21  0.35    1.10  0.78
 138    0.96  0.76   0.18           1.12  1.80    0.61  1.02    3.15  2.25

 118       0.70     TRIBUTYLAMINE 75649
 100    0.42  0.33   0.08           0.49  0.75    0.27  0.44    0.97  0.69
 142    1.53  1.18   0.28           1.77  2.74    0.97  1.61    3.52  2.51

 119       0.92     CAFFEINE 58082
 109    0.10  0.08   0.02           0.12  0.17    0.06  0.10    0.23  0.16
 194    0.19  0.15   0.04           0.22  0.34    0.12  0.20    0.44  0.32

 120       0.62     DIBENZYLAMINE 103491
  91    1.62  1.26   0.30           1.78  2.87    1.16  1.94    3.63  2.67
 197    0.13  0.11   0.03           0.15  0.24    0.10  0.16    0.30  0.22

 121       0.68     N,N-DIMETHYLDODECYLAMINE 112185
  58    4.72  3.88   0.87           5.47  8.83    3.58  5.99   11.09  8.16
  59    0.17  0.13   0.03           0.20  0.30    0.13  0.21    0.40  0.29

 122       0.90     ATRAZINE 1912249
 200    2.75  2.20   0.52           3.28  5.23    1.72  2.86    8.17  6.09
 215    1.67  1.34   0.31           2.00  3.18    1.05  1.74    4.97  3.71
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           Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery   Compound Name
           Std #59      Std #60      Std #61         Std #62          Std #63
Mass     110   125     82   110     264      -      188      -        99     -


 110       0.01      P-NITROANILINE 100016
  65    0.34  1.13    0.49  0.19    0.14             0.04             0.51
 138    0.43  1.84    0.62  0.24    0.19             0.05             0.65

 111       0.80      2,4-DIMETHYLQUINOLINE 1198374
 156    0.29  0.96    0.40  0.15    0.15             0.03             0.43
 157    1.46  4.69    1.93  0.74    0.71             0.15             2.09

 112       0.01      1,8-DIAMINONAPHTHALENE 569415
 114    0.02  0.08    0.03  0.01    0.01             0.00             0.03
 141    0.04  0.12    0.05  0.02    0.01             0.00             0.55

 113       0.84      NICOTINE 54115
  84    0.82  2.74    1.12  0.43    0.41             0.09             1.22
 133    0.19  0.64    0.26  0.10    0.10             0.02             0.29

 114       0.79      CARBAZOLE 86748
 167    2.60  8.72    3.57  1.37    1.28             0.31             4.22

 115       0.91      2-AMINOBIPHENYL 90445
 168    4.75 16.46    7.10  2.75    2.13             0.51             7.45
 169    8.82 30.44   13.14  5.08    3.96             0.95            13.80

 116       0.76      DIPHENYLAMINE 122394
 168    1.03  3.47    1.42  0.55    0.52             0.11             1.55
 169    1.94  6.46    2.68  1.03    0.98             0.22             2.91

 117       0.01      DICYCLOHEXYLAMINE 101837
  56    0.25  0.81    0.33  0.14    0.09             0.03             0.38
 138    0.71  2.34    0.95  0.40    0.26             0.08             1.09

 118       0.70      TRIBUTYLAMINE 75649
 100    0.29  0.99    0.41  0.16    0.15             0.03             0.44
 142    0.99  3.34    1.47  0.57    0.53             0.12             1.59

 119       0.92      CAFFEINE 58082
 109    0.07  0.23    0.09  0.04    0.04             0.01             0.10
 194    0.13  0.45    0.18  0.07    0.07             0.02             0.21

 120       0.62      DIBENZYLAMINE 103491
  91    1.18  3.91    1.52  0.59    0.62             0.11             1.74
 197    0.10  0.32    0.13  0.05    0.05             0.01             0.14

 121       0.68      N,N-DIMETHYLDODECYLAMINE 112185
  58    3.62 12.02    4.66  1.81    1.87             0.34             5.37
  59    0.13  0.43    0.17  0.06    0.07             0.01             0.19

 122       0.90      ATRAZINE 1912249
 200    2.13  7.07    3.05  1.18    0.90             0.22             3.26
 215    1.21  4.30    1.85  0.72    0.55             0.13             1.95
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Internal/External Standard File for Cmpd Class # 3

Cmpd#	Recovery		Compound Name							
	Std # 2		Std #54		Std #56		Std #57		Std #58	
Mass	109	236	136	-	82	128	98	116	84	112
123	0.01		HEPTANONE 110430							
43	1.21	0.94	0.22		1.33	2.14	0.85	1.14	2.32	2.00
58	0.75	0.58	0.14		0.83	1.33	0.53	0.88	1.69	1.25
124	0.65		BUTOXYETHANOL 111762							
41	0.21	0.17	0.04		0.25	0.40	0.13	0.22	0.49	0.35
57	0.55	0.42	0.10		0.63	1.03	0.35	0.58	1.27	0.91
125	0.70		2-OCTANONE 111137							
43	1.30	1.01	0.24		1.43	2.31	0.91	1.53	2.92	2.15
58	1.02	0.79	0.19		1.11	1.80	0.71	1.19	2.27	1.67
126	0.61		BUTYLPROPIONATE 590012							
57	1.48	1.14	0.27		1.71	2.73	0.90	1.49	4.27	3.15
75	0.44	0.34	0.08		0.51	0.82	0.27	0.45	1.28	0.95
127	0.78		ISOPHORONE 78591							
82	1.77	1.36	0.33		2.04	3.17	1.13	1.86	4.11	2.93
138	0.39	0.30	0.07		0.45	0.72	0.25	0.41	0.90	0.64
128	0.74		FENCHONE 1195759							
69	0.66	0.51	0.12		0.72	1.17	0.47	0.78	1.47	1.08
81	1.44	1.12	0.27		1.58	2.55	1.02	1.71	3.22	2.36
129	0.75		ALPHA-TERPINEOL 98555							
59	0.56	0.43	0.10		0.65	1.00	0.36	0.59	1.31	0.93
136	0.32	0.25	0.06		0.37	0.58	0.21	0.34	0.75	0.53
130	0.95		N-DECANOL 112301							
41	0.40	0.31	0.07		0.46	0.74	0.25	0.42	0.92	0.66
43	0.44	0.34	0.08		0.51	0.79	0.28	0.46	1.02	0.73
131	0.62		DIMETHYLADIPATE 627930							
59	0.56	0.45	0.10		0.64	1.03	0.41	0.69	1.29	0.95
114	0.44	0.35	0.08		0.49	0.79	0.32	0.54	1.00	0.74
132	0.77		METHYLSTEARATE 112618							
74	3.42	2.65	0.63		3.89	6.28	2.54	4.25	7.90	5.81
87	2.22	1.72	0.41		2.52	4.07	1.65	2.76	5.13	3.77
133	0.64		N-DECANE 124185							
43	1.47	1.11	0.26		1.67	2.66	0.88	1.46	4.18	3.09
57	1.42	1.08	0.25		1.64	2.61	0.85	1.41	4.05	3.00
134	0.66		N-TRIDECANE 629505							
43	2.18	1.64	0.34		2.48	3.95	1.30	2.16	6.20	4.58
57	2.75	2.09	0.50		3.14	5.01	1.66	2.77	7.93	5.86
135	0.48		N-TETRADECANE 629594							
43	2.52	1.92	0.45		2.88	4.58	1.51	2.51	7.19	5.31
57	3.40	2.55	0.61		3.87	6.16	2.03	3.37	9.67	7.15

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            Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery    Compound Name
          Std #59       Std #60        Std #61          Std #62          Std #63
Mass     110   125      82    110      264     -        188     -        99     -


 123        0.01     HEPTANONE 110430
  43     0.88  2.91    1.13  0.44    0.47             0.08             1.30
  58     0.55  1.82    0.71  0.27    0.29             0.05             0.81

 124        0.65     BUTOXYETHANOL 111762
  41     0.15  0.49    0.20  0.09    0.07             0.02             0.22
  57     0.38  1.28    0.52  0.20    0.19             0.04             0.57

 125        0.70     2-OCTANONE 111137
  43     0.95  3.14    1.22  0.47    0.51             0.09             1.40
  58     0.74  2.45    0.95  0.37    0.39             0.07             1.09

 126        0.61     BUTYLPROPIONATE 590012
  57     1.11  3.69    1.59  0.61    0.48             0.12             1.66
  75     0.33  1.11    0.48  0.19    0.15             0.04             0.50

 127        0.78     ISOPHORONE 78591
  82     1.23  4.14    1.70  0.65    0.62             0.14             1.80
 138     0.27  0.91    0.37  0.14    0.14             0.03             0.41

 128        0.74     FENCHONE 1195759
  69     0.48  1.58    0.62  0.24    0.25             0.05             0.71
  81     1.05  3.45    1.35  0.52    0.55             0.10             1.55

 129        0.75     ALPHA-TERPINEOL 98555
  59     0.39  1.31    0.54  0.21    0.20             0.04             0.58
 136     0.23  0.76    0.31  0.12    0.11             0.03             0.34

 130        0.95     N-DECANOL 112301
  41     0.28  0.93    0.38  0.15    0.14             0.03             0.41
  43     0.31  1.63    0.42  0.16    0.15             0.03             0.46

 131        0.62     DIMETHYLADIPATE 627930
  59     0.42  1.40    0.54  0.21    0.22             0.04             0.62
 114     0.33  1.08    0.42  0.16    0.17             0.03             0.48

 132        0.77     METHYLSTEARATE 112618
  74     2.58  8.56    3.32  1.29    1.33             0.24             3.83
  87     1.67  5.55    2.15  0.83    0.87             0.16             2.48

 133        0.64     N-DECANE 124185
  43     1.05  3.59    1.55  0.60    0.47             0.11             1.62
  57     1.01  3.48    1.50  0.58    0.46             0.11             1.58

 134        0.66     N-TRIDECANE 629505
  43     1.56  5.33    2.30  0.89    0.70             0.17             2.41
  57     1.99  6.75    2.94  1.14    0.76             0.21             3.09

 135        0.48     N-TETRADECANE 629594
  43     1.86  6.19    2.67  1.03    0.80             0.19             2.80
  57     2.50  8.33    3.57  1.39    1.08             0.26             3.77
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              Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56       Std #57       Std #58
Mass     109   236    136    -      82    128     98    116     84    112


 136       0.68     N-PENTADECANE 692629
  57    2.78  2.14   0.52          3.22  4.99    1.77  2.94    6.47  4.62
  71    1.73  1.33   0.32          2.01  3.11    1.10  1.83    4.03  2.87

 137       0.51     N-HEXADECANE 544763
  43    1.90  1.45   0.34          2.16  3.45    1.13  1.89    5.41  3.99
  57    2.72  2.08   0.49          3.11  4.96    1.63  2.71    7.78  5.74

 138       0.78     N-HEPTADECANE 629787
  57    3.13  2.41   0.58          3.61  5.59    1.99  3.30    7.25  5.17
  71    2.07  1.60   0.38          2.39  3.70    1.32  2.18    4.80  3.42

 139       0.67     N-OCTADECANE 593453
  57    2.99  2.51   0.59          3.75  5.98    1.88  3.14    8.96  6.63
  71    1.98  1.66   0.39          2.48  3.95    1.25  2.08    5.95  4.41

 140       0.63     N-NONADECANE 629925
  71    2.12  1.61   0.38          2.42  3.85    1.27  2.11    6.04  4.47
  85    1.42  1.08   0.25          1.61  2.57    0.85  1.41    4.03  2.98

 141       0.75     N-EICOSANE 1112958
  57    4.43  3.41   0.82          5.11  7.92    2.82  4.66   10.26  7.32
  71    3.03  2.33   0.56          3.50  5.43    1.93  3.19    7.03  5.01

 142       0.66     N-HENEICOSANE 629947
  57    3.93  2.96   0.70          4.43  7.05    2.32  3.86   11.05  8.20
  71    2.71  2.05   0.48          3.07  4.88    1.61  2.67    7.65  5.68

 143       0.64     N-DOCOSANE 629970
  57    3.73  2.98   0.70          4.46  7.10    2.33  3.88   11.11  8.26
  71    2.60  2.08   0.49          3.11  4.96    1.63  2.70    7.76  5.77

 144       0.65     N-TRICOSANE 638675
  57    3.99  3.19   0.75          4.77  7.60    2.49  4.14   11.85  8.83
  71    2.80  2.24   0.53          3.35  5.34    1.75  2.91    8.33  6.20

 145       0.01     PHENYLACETATE 122792
  94    1.84  1.43   0.34          2.01  3.25    1.30  2.18    4.10  3.01
 136    0.25  0.20   0.04          0.28  0.45    0.18  0.30    0.57  0.42

 146       0.74     BENZYLACETATE 140114
  91    0.52  0.40   0.09          0.57  0.92    0.37  0.62    1.15  0.85
 108    1.09  0.85   0.20          1.19  1.92    0.77  1.29    2.43  1.79

 147       0.81     METHYLBENZENESULFONATE
  77    1.24  0.94   0.22          1.41  2.25    0.74  1.23    3.54  2.61
 172    0.44  0.34   0.08          0.50  0.80    0.26  0.44    1.26  0.93

 148       0.67     METHYLTOLUENESULFONATE
  91    1.60  1.21   0.29          1.81  2.89    0.95  1.58    4.53  3.35
 155    0.72  0.54   0.13          0.81  1.29    0.42  0.71    2.02  1.50
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              Internal/External Standard File for Cmpd Class # 3

Cmpd#     Recovery    Compound Name
           Std #59       Std #60       Std #61          Std #62          Std #63
Mass      110   125     82   110      264    -         188    -          99    -


  136       0.68      N-PENTADECANE 692629
   57    1.94  6.52    2.68  1.03    0.99             0.22              2.92
   71    1.21  4.06    1.67  0.64    0.62             0.14              1.82

  137       0.51      N-HEXADECANE 544763
   43    1.40  4.66    2.01  0.78    0.61             0.15              2.11
   57    2.01  6.70    2.88  1.12    0.87             0.21              3.03

  138       0.78      N-HEPTADECANE 629787
   57    2.18  7.32    3.01  1.16    1.11             0.24              3.27
   71    1.44  4.85    1.99  0.77    0.73             0.16              2.17

  139       0.67      N-OCTADECANE 593453
   57    2.33  8.10    3.48  1.35    1.01             0.24              3.65
   71    1.55  5.35    2.30  0.89    0.58             0.06              2.41

  140       0.63      N-NONADECANE 629925
   71    1.51  5.27    2.24  0.87    0.68             0.16              2.35
   85    1.01  3.47    1.50  0.58    0.45             0.11              1.57

  141       0.75      N-EICOSANE 1112958
   57    3.08 10.35    4.25  1.63    1.57             0.35              4.63
   71    2.11  7.09    2.91  1.12    1.07             0.23              3.17

  142       0.66      N-HENEICOSANE 629947
   57    2.73  9.53    4.11  1.60    1.07             0.30              4.31
   71    1.89  6.60    2.85  1.10    0.74             0.21              2.99

  143       0.64      N-DOCOSANE 629970
   57    2.89  9.60    4.14  1.60    1.22             0.30              4.35
   71    2.02  6.71    2.89  1.12    0.85             0.21              3.04

  144       0.65      N-TRICOSANE 638675
   57    3.10 10.28    4.42  1.71    1.29             0.32              4.65
   71    2.18  7.22    3.11  1.20    0.90             0.22              3.27

  145       0.01      PHENYLACETATE 122792
   94    1.31  4.43    1.72  0.67    0.70             0.13              1.98
  136    0.18  0.62    0.24  0.09    0.10             0.02              0.28

  146       0.74      BENZYLACETATE 140114
   91    0.38  1.25    0.48  0.19    0.20             0.04              0.56
  108    0.79  2.63    1.02  0.40    0.41             0.07              1.17

  147       0.81      METHYLBENZENESULFONATE
   77    0.91  3.04    1.31  0.51    0.40             0.09              1.38
  172    0.32  1.08    0.47  0.18    0.14             0.03              0.49

  148       0.67      METHYLTOLUENESULFONATE
   91    1.17  3.90    1.68  0.65    0.51             0.12              1.76
  155    0.52  1.74    0.75  0.29    0.23             0.05              0.79
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                 Internal/External Standard File for Cmpd Class # 3

Cmpd#     Recovery    Compound Name
           Std # 2      Std #54        Std #56       Std #57       Std #58
Mass      109   236    136    -       82    128     98    116     84    112


  149       1.07      DIMETHYLPHTHALATE 131113
   77    0.81  0.63    0.15          0.94  1.45    0.52  0.85    1.88  1.34
  163    5.29  4.07    0.98          6.10  9.46    3.36  5.56   12.22  8.71

  150       0.91      ETHYLTOLUENESULFONATE
   91    1.74  1.32    0.31          1.97  3.14    1.03  1.72    4.92  3.65
  155    1.18  0.94    0.22          1.40  2.23    0.73  1.21    3.46  2.35

  151       1.08      DIETHYLPHTHALATE 84662
  149    3.19  2.43    0.57          3.65  5.79    1.90  3.17    9.08  6.71
  177    0.80  0.61    0.14          0.93  1.47    0.48  0.80    2.29  1.69

  152       0.96      DIBUTYLPHTHALATE 84742
   57    0.29  0.23    0.05          0.34  0.52    0.19  0.31    0.68  0.48
  149    7.17  5.52    1.33          8.27 12.80    4.55  7.54   16.55 11.80

  153       0.97      BUTYLBENZYLPHTHALATE
   91    2.09  1.62    0.38          2.28  3.69    1.48  2.48    4.64  3.41
  149    3.37  2.62    0.62          3.69  5.95    2.40  4.01    7.49  5.51

  154       1.02      DIETHYLHEXYLPHTHALATE 117817
  149    5.22  4.07    0.96          5.71  9.23    3.74  6.26   11.59  8.53
  167    1.98  1.54    0.37          2.17  3.51    1.42  2.37    4.40  3.24

  155       0.89      BENZALDEHYDE 100527
   77    0.36  0.28    0.07          0.42  0.64    0.23  0.38    0.84  0.66
  105    0.40  0.31    0.07          0.46  0.70    0.25  0.42    0.92  0.66

  156       0.66      TOLUALDEHYDE 529204
   91    0.54  0.44    0.10          0.65  1.04    0.34  0.57    1.65  1.21
  119    0.63  0.51    0.12          0.77  1.23    0.41  0.68    1.95  1.43

  157       0.87      ACETOPHENONE 98862
   77    0.38  0.64    0.15          0.96  1.53    0.53  0.87    1.93  1.37
  105    1.22  0.94    0.23          1.41  2.25    0.78  1.29    2.85  2.03

  158       0.73      SALICYLALDEHYDE 90028
  121    0.56  0.44    0.10          0.61  0.99    0.40  0.67    1.24  0.91
  122    0.60  0.47    0.11          0.60  1.07    0.43  0.72    1.34  0.99

  159       0.72      ANISALDEHYDE 123115
  135    1.37  1.08    0.25          1.53  2.47    0.91  1.66    3.11  2.29
  136    0.96  0.76    0.18          1.07  1.73    0.70  1.16    2.18  1.60

  160       0.85      PHENOL 108952
   94    1.07  0.84    0.20          1.18  1.90    0.76  1.27    2.41  1.77

  161       0.72      CRESOL 108394
  107    1.21  0.93    0.23          1.40  2.25    0.80  1.29    2.91  2.08
  108    1.07  0.82    0.20          1.24  1.99    0.69  1.14    2.58  1.84
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             Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery   Compound Name
          Std #59       Std #60       Std #61        Std #62        Std #63
Mass     110   125     82   110     264     -      188     -        99     -


 149       1.07      DIMETHYLPHTHALATE 131113
  77    0.57  1.83    0.75  0.29    0.28           0.06           0.85
 163    3.68 11.87    4.88  1.88    1.85           0.41           5.51

 150       0.91      ETHYLTOLUENESULFONATE
  91    1.28  4.25    1.83  0.71    0.55           0.13           1.92
 155    0.91  3.01    1.30  0.50    0.38           0.09           1.36

 151       1.08      DIETHYLPHTHALATE 84662
 149    2.35  7.82    3.34  1.30    1.02           0.24           3.54
 177    0.59  1.97    0.85  0.33    0.26           0.06           0.89

 152       0.96      DIBUTYLPHTHALATE 84742
  57    0.20  0.68    0.28  0.11    0.10           0.02           0.31
 149    4.99 16.75    6.88  2.64    2.52           0.55           7.47

 153       0.97      BUTYLBENZYLPHTHALATE
  91    1.51  5.02    1.95  0.76    0.78           0.14           2.24
 149    2.44  8.10    3.15  1.22    1.26           0.23           3.62

 154       1.02      DIETHYLHEXYLPHTHALATE 117817
 149    4.03 12.58    4.88  1.89    1.90           0.35           5.61
 167    1.53  4.78    1.85  0.72    0.72           0.13           2.13

 155       0.89      BENZALDEHYDE 100527
  77    0.25  0.84    0.35  0.13    0.13           0.03           0.38
 105    0.28  0.93    0.38  0.15    0.14           0.03           0.42

 156       0.66      TOLUALDEHYDE 529204
  91    0.42  1.41    0.61  0.24    0.15           0.05           0.64
 119    0.50  1.66    0.72  0.28    0.22           0.05           0.75

 157       0.87      ACETOPHENONE 98862
  77    0.57  1.95    0.80  0.31    0.29           0.06           0.87
 105    0.85  2.88    1.18  0.45    0.43           0.09           1.28

 158       0.73      SALICYLALDEHYDE 90028
 121    0.41  1.35    0.52  0.20    0.21           0.04           0.60
 122    0.44  1.46    0.56  0.22    0.23           0.04           0.65

 159       0.72      ANISALDEHYDE 123115
 135    1.01  3.36    1.30  0.51    0.53           0.09           1.50
 136    0.71  2.36    0.91  0.35    0.37           0.07           1.05

 160       0.85      PHENOL 108952
  94    0.75  2.60    1.01  0.39    0.41           0.07           1.15

 161       0.72      CRESOL 108394
 107    0.88  2.85    1.17  0.45    0.44           0.10           1.31
 108    0.78  2.52    1.03  0.40    0.39           0.09           1.16
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              Internal/External Standard File for Cmpd Class # 3

Cmpd#     Recovery    Compound Name
           Std # 2     Std #54         Std #56        Std #57         Std #58
Mass      109    236   136     -        82   128       98    116       84    112


 162       0.01       2,3-DIMETHYLPHENOL 526750
 107     0.87   0.67   0.16           1.00  1.61     0.57  0.95      2.08  1.48
 122     0.91   0.70   0.17           1.05  1.64     0.58  0.96      2.12  1.51

 163       0.74       ISOPROPYLPHENOL(O) 88699
 121     1.79   1.36   0.32           2.04  3.25     1.07  1.78      5.10  3.77
 136     0.07   0.56   0.12           0.75  1.19     0.39  0.65      1.87  1.38

 164       0.01       O-NITROPHENOL 88755
  65     0.03   0.02   0.00           0.03  0.05     0.02  0.03      0.06  0.05
 139     0.13   0.10   0.02           0.14  0.23     0.09  0.15      0.29  0.21

 165       0.98       4-CHLORO-3-METHYLPHENOL 59507
 107     0.93   0.71   0.17           1.06  1.68     0.55  0.92      2.64  2.95
 142     1.02   0.77   0.18           1.16  1.84     0.61  1.01      2.89  2.14

 166       0.01       4-CHLOROCRESOL 59507 OR 1570645
 107     0.83   0.64   0.16           0.97  1.57     0.53  0.88      2.03  1.45
 142     0.94   0.72   0.17           1.09  1.77     0.60  0.99      2.29  1.63

 167       0.01       1-NAPHTHOL 90153
 115     0.35   0.26   0.06           0.38  0.61     0.20  0.34      0.96  0.72
 144     0.61   0.45   0.11           0.67  1.07     0.35  0.29      1.68  1.25

 168       0.80       P-TERT-BUTYLPHENOL 98544
 107     0.56   0.43   0.10           0.65  1.03     0.34  0.56      1.60  1.18
 135     1.96   1.49   0.35           2.22  3.54     1.17  1.94      5.56  4.11

 169       0.76       2-NITROCRESOL 119335
  77     0.26   0.20   0.05           0.30  0.46     0.07  0.27      0.60  0.43
 153     0.74   0.57   0.14           0.83  1.33     0.46  0.78      1.72  1.23

 170       0.01       2,4-DICHLOROPHENOL 120832
 162     1.13   0.88   0.21           1.24  2.00     0.80  1.34      2.52  1.86
 164     0.72   0.53   0.13           0.78  1.27     0.51  0.85      1.60  1.18

 171       0.01       2,4,6-TRICHLOROPHENOL 88062
 196     0.81   0.63   0.15           0.89  1.44     0.58  0.97      1.88  1.34
 198     0.83   0.64   0.15           0.91  1.46     0.59  0.98      1.90  1.36

 172       0.01       DI-TERT-BUTYL-4-METHYLPHENOL 128370
 205     2.53   1.97   0.47           2.78  4.49     1.81  3.03      5.66  4.16
 220     0.67   0.52   0.12           0.73  1.18     0.48  0.80      1.49  1.09

 173       0.01       PENTACHLOROPHENOL 87865
 264     0.29   0.22   0.05           0.34  0.54     0.19  0.31      0.72  0.52
 266     0.47   0.36   0.09           0.55  0.91     0.32  0.54      1.17  0.84

 174       0.71       2-METHYLNAPHTHALENE 91576
 141     2.03   1.58   0.38           2.23  3.60     1.44  2.42      4.53  3.34
 142     2.51   1.96   0.46           2.76  4.45     1.79  2.99      5.62  4.13
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            Internal/External Standard File for Cmpd Class # 3

 Cmpd#     Recovery    Compound Name
            Std #59      Std #60       Std #61       Std #62       Std #63
 Mass      110   125     82    110    264     -     188     -      99     -


  162       0.01       2,3-DIMETHYLPHENOL 526750
  107     0.63  2.11    0.84  0.32    0.32          0.07          0.94
  122     0.64  2.14    0.85  0.33    0.32          0.07          0.95

  163       0.74       ISOPROPYLPHENOL(O) 88699
  121     1.28  4.39    1.90  0.73    0.58          0.14          1.99
  136     0.47  1.61    0.69  0.27    0.21          0.05          0.73

  164       0.01       O-NITROPHENOL 88755
   65     0.02  0.07    0.03  0.01    0.01          0.00          0.03
  139     0.09  0.31    0.12  0.05    0.05          0.01          0.14

  165       0.98       4-CHLORO-3-METHYLPHENOL 59507
  107     0.66  2.26    0.98  0.38    0.30          0.07          1.03
  142     0.72  2.49    1.07  0.42    0.32          0.08          1.13

  166       0.01       4-CHLOROCRESOL 59507 OR 1570645
  107     0.58  1.96    0.80  0.31    0.31          0.07          0.91
  142     0.66  2.20    0.85  0.34    0.35          0.08          1.03

  167       0.01       1-NAPHTHOL 90153
  115     0.25  0.83    0.36  0.14    0.11          0.03          0.38
  144     0.44  1.45    0.62  0.24    0.18          0.05          0.66

  168       0.80       P-TERT-BUTYLPHENOL 98544
  107     0.40  1.38    0.66  0.23    0.18          0.04          0.62
  135     1.44  4.79    2.04  0.80    0.63          0.15          2.16

  169       0.76       2-NITROCRESOL 119335
   77     0.18  0.61    0.25  0.10    0.09          0.02          0.27
  153     0.52  1.74    0.71  0.27    0.26          0.06          0.78

  170       0.01       2,4-DICHLOROPHENOL 120832
  162     0.80  2.73    1.05  0.41    0.43          0.08          1.22
  164     0.51  1.70    0.67  0.26    0.27          0.05          0.77

  171       0.01       2,4,6-TRICHLOROPHENOL 88062
  196     0.58  1.97    0.76  0.30    0.91          0.05          0.88
  198     0.58  1.99    0.77  0.30    0.32          0.06          0.89

  172       0.01       DI-TERT-BUTYL-4-METHYLPHENOL 128370
  205     1.85  6.13    2.37  0.92    0.96          0.17          2.73
  220     0.49  1.61    0.62  0.24    0.25          0.05          0.72

  173       0.01       PENTACHLOROPHENOL 87865
  264     0.20  0.68    0.28  0.11    0.11          0.02          0.31
  266     0.36  1.11    0.45  0.07    0.18          0.04          0.50

  174       0.71       2-METHYLNAPHTHALENE 91576
  141     1.48  4.91    1.90  0.74    0.77          0.14          2.19
  142     1.78  6.08    2.36  0.91    0.95          0.17          2.71
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              Internal/External Standard File for Cmpd Class # 3

Cmpd#     Recovery    Compound Name
           Std # 2      Std #54       Std #56       Std #57       Std #58
Mass      109   236    136    -       82   128      98   116      84   112


 175        0.78      ACENAPHTHENE 83329
 153     1.26  0.98    0.23          1.38  2.22    0.89  1.49    2.81  2.06
 154     3.40  2.64    0.63          3.73  6.02    2.41  4.04    7.59  5.58

 176        0.80      BIPHENYL 92524
 154     2.28  1.78    0.42          2.51  4.04    1.63  2.72    5.10  3.75

 177        0.71      1,8-DIMETHYLNAPHTHALENE 569415
 141     1.59  1.24    0.29          1.74  2.82    1.13  1.89    3.55  2.61
 156     2.30  1.79    0.42          2.52  4.07    1.63  2.73    5.13  3.77

 178        0.85      FLUORENE 86737
 165     2.74  2.13    0.49          3.01  4.85    1.95  3.27    6.12  4.50
 166     3.07  2.38    0.57          3.44  5.55    2.23  3.74    6.99  5.14

 179        0.74      2,3,5-TRIMETHYLNAPHTHALENE 2245387
 155     1.86  1.44    0.34          2.08  3.36    1.36  2.27    4.24  3.12
 170     2.56  1.99    0.47          2.86  4.62    1.86  3.11    5.83  4.29

 180        0.01      ANTHRACENE 120127
 178     3.21  2.47    0.60          3.71  5.74    2.04  3.38    7.43  5.30

 181        0.80      PYRENE 129000
 202     4.88  3.75    0.95          5.66  8.73    3.27  5.18   11.54  8.23

 182        0.45      9,10-DIMETHYLANTHRACENE 781431
 191     1.33  1.03    0.25          1.45  2.35    0.94  1.57    2.96  2.18
 206     2.85  2.22    0.53          3.13  5.04    2.01  3.37    6.36  4.68

 183        0.78      CHRYSENE 218019
 228     2.21  1.73    0.41          2.42  3.92    1.59  2.66    4.91  3.61

 184        0.54      PERYLENE 198550
 252     1.60  1.23    0.30          1.84  2.86    1.02  1.68    3.67  2.62

 185        1.35      DICYANOBUTANE 111693
  41     0.66  0.51    0.12          0.72  1.17    0.47  0.79    1.47  1.08
  54     0.29  0.23    0.05          0.32  0.52    2.10  0.35    0.66  0.48

 186        0.60      BUTYLCARBAMATE  14994775
  41     0.48  0.36    0.08          0.54  0.86    0.28  0.47    1.35  1.00
  59     0.24  0.26    0.05          0.29  0.47    0.15  0.25    0.72  0.54

 187        0.01      DIBUTYLDISULFIDE 110065
  41     0.73  0.56    0.13          0.84  1.34    0.44  0.73    2.10  1.55
  57     3.09  2.36    0.56          3.54  5.64    1.85  3.09    8.84  6.54

 188        0.78      BIS(2-CHLOROETHYL)ETHANE 112265
  63     1.71  1.31    0.31          1.97  3.13    1.03  1.71    4.91  3.63
  93     0.84  0.65    0.15          0.97  1.54    0.51  0.84    2.42  1.78
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           Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery    Compound Name
          Std #59       Std #60      Std #61       Std #62       Std #63
Mass      110   125      82   110     264    -      188    -       99    -


 175        0.78     ACENAPHTHENE 83329
 153     0.92  3.04   1.18  0.46    0.47          0.09           1.35
 154     2.48  8.22   3.19  1.23    1.28          0.23           3.66

 176        0.80     BIPHENYL 92524
 154     1.67  5.52   2.14  0.83    0.87          0.16           2.46

 177        0.71     1,8-DIMETHYLNAPHTHALENE 569415
 141     1.16  3.84   1.49  0.58    0.60          0.11           1.71
 156     1.67  5.55   2.15  0.83    0.87          0.16           2.48

 178        0.85     FLUORENE 86737
 165     2.00  6.62   2.57  0.99    1.04          0.19           2.95
 166     2.28  7.57   2.93  1.14    1.19          0.21           3.38

 179        0.74     2,3,5-TRIMETHYLNAPHTHALENE 2245387
 155     1.38  4.59   1.78  0.69    0.72          0.13           2.05
 170     1.90  6.31   2.44  0.95    0.99          0.18           2.81

 180        0.01     ANTHRACENE 120127
 178     2.24  7.59   3.08  1.19    1.13          0.25           3.35

 181        0.80     PYRENE 129000
 202     3.59 11.47   4.95  1.90    1.80          0.40           5.36

 182        0.45     9,10-DIMETHYLANTHRACENE 781431
 191     0.96  3.19   1.24  0.48    0.50          0.09           1.42
 206     2.06  6.86   2.67  1.03    1.08          0.19           3.06

 183        0.78     CHRYSENE 218019
 228     1.61  5.34   2.07  0.80    0.81          0.15           2.39

 184        0.54     PERYLENE 198550
 252     1.11  3.72   1.53  0.59    0.47          0.12           1.65

 185        1.35     DICYANOBUTANE 111693
  41     0.48  1.59   0.62  0.24    0.25          0.05           0.71
  54     0.22  0.71   0.28  0.11    0.11          0.02           0.32

 186        0.60     BUTYLCARBAMATE  14994775
  41     0.35  1.16   0.50  0.09    0.15          0.04           0.52
  59     0.19  0.63   0.27  0.11    0.08          0.02           0.28

 187        0.01     DIBUTYLDISULFIDE 110065
  41     0.54  1.78   0.78  0.31    0.20          0.06           0.82
  57     2.21  7.62   3.29  1.27    1.00          0.24           3.42

 188        0.78     BIS(2-CHLOROETHYL)ETHANE 112265
  63     1.27  4.23   1.83  0.71    0.56          0.13           1.91
  93     0.61  2.08   0.90  0.35    0.27          0.06           0.94
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            Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery    Compound Name
          Std # 2     Std #54      Std #56      Std #57      Std #58
Mass     109   236   136    -     82   128     98   116     84   112


 189       0.93     TRIBUTYLPHOSPHATE 126738
  99    4.03  3.10   0.75         4.65  7.20   2.56  4.24   9.28  6.62
 155    0.88  0.68   0.16         1.01  1.57   0.56  0.92   2.02  1.44

 190       0.01     ALDRIN 309002
  66    1.33  1.03   0.24         1.49  2.40   0.97  1.62   3.03  2.23
 263    0.60  0.46   0.11         0.67  1.08   0.44  0.73   1.36  1.00

 191       0.67     DIHYDROBENZOFURAN 496162
  91    0.68  0.52   0.13         0.79  1.25   0.43  0.72   1.58  1.13
 120    0.97  0.75   0.18         1.12  1.67   0.66  0.78   2.16  1.54

 192       0.86     NITROBENZENE 98953
  77    0.86  0.67   0.16         0.94  1.51   0.61  1.02   1.91  1.40
 123    0.54  0.42   0.10         0.59  0.95   0.38  0.64   1.20  0.88

 193       0.71     BENZOTHIAZOLE 95169
 135    1.56  1.21   0.29         1.71  2.76   1.11  1.86   3.47  2.55

 194       0.01     PHENYLCARBAMATE 102090
  94    1.25  0.96   0.23         1.44  2.23   0.79  1.31   2.88  2.06
 137    0.02  0.01   0.00         0.02  0.03   0.01  0.02   0.04  0.03

 195       0.01     2,4-DINITROTOLUENE 121142
  89    0.35  0.28   0.06         0.40  0.65   0.26  0.44   0.81  0.60
 165    0.71  0.53   0.13         0.75  1.21   0.46  0.76   1.53  1.13

 196       0.84     BENZYLSULFIDE 538749
  91    3.55  2.68   0.63         4.00  6.38   2.10  3.49   9.99  7.42
 123    0.90  0.68   0.16         1.02  1.62   0.53  0.89   2.54  1.88

 197       0.86     DIPHENYLSULFONE 127639
 125    3.82  3.44   0.81         5.16  8.21   2.71  4.51  12.95  8.65
 218    0.92  0.73   0.17         1.10  1.75   0.58  0.96   2.74  2.03

 198       0.93     TRIPHENYLPHOSPHATE 115866
 325    2.59  2.01   0.13         0.79  1.28   0.52  0.87   1.61  1.18
 326    0.09  0.07   0.17         1.03  1.67   0.68  1.14   2.09  1.54

 199       1.12     DIPHENYLMERCURY 587859
  77    0.72  0.56   0.48         2.85  4.59   1.96  3.28   6.08  4.47
 356    0.95  0.74   0.02         0.09  0.15   0.06  0.11   0.20  0.15

 200       0.94     TETRAPHENYLTIN
 197    1.40  1.13   0.27         1.70  2.71   0.89  1.47   4.21  3.13
 351    1.30  1.05   0.25         1.58  2.51   0.82  1.37   3.91  2.91

 201       0.63     BENZYLCHLORIDE 100447
  91    1.55  1.18   0.28         1.77  2.82   0.93  1.54   4.42  3.28
 126    0.42  0.32   0.08         0.48  0.76   0.25  0.42   1.20  0.89
```

```
        Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery   Compound Name
          Std #59      Std #60      Std #61       Std #62       Std #63
Mass     110   125     82   110    264    -      188    -       99    -


 189       0.93     TRIBUTYLPHOSPHATE 126738
  99    2.81  9.43   3.87  1.49   1.41           0.31           4.19
 155    0.61  2.05   0.84  0.32   0.31           0.07           0.91

 190       0.01     ALDRIN 309002
  66    0.99  3.28   1.27  0.49   0.51           0.09           1.46
 263    0.44  1.47   0.57  0.22   0.23           0.04           0.66

 191       0.67     DIHYDROBENZOFURAN 496162
  91    0.27  1.59   0.65  0.25   0.24           0.05           0.71
 120    0.68  2.27   0.90  0.35   0.33           0.07           0.98

 192       0.86     NITROBENZENE 98953
  77    0.61  2.07   0.80  0.31   0.33           0.06           0.94
 123    0.38  1.30   0.50  0.20   0.21           0.04           0.59

 193       0.71     BENZOTHIAZOLE 95169
 135    1.14  3.76   1.46  0.57   0.59           0.11           1.68

 194       0.01     PHENYLCARBAMATE 102090
  94    0.87  2.92   1.20  0.46   0.44           0.10           1.30
 137    0.01  0.04   0.01  0.01   0.00           0.00           0.02

 195       0.01     2,4-DINITROTOLUENE 121142
  89    0.27  0.88   0.34  0.13   0.14           0.03           0.39
 165    0.50  1.66   0.64  0.25   0.26           0.05           0.74

 196       0.84     BENZYLSULFIDE 538749
  91    2.47  8.62   3.72  1.44   1.11           0.27           3.90
 123    0.63  2.19   0.94  0.37   0.28           0.07           0.99

 197       0.86     DIPHENYLSULFONE 127639
 125    3.00 11.09   4.77  1.85   1.22           0.35           5.05
 218    0.67  2.36   1.02  0.29   0.30           0.07           1.07

 198       0.93     TRIPHENYLPHOSPHATE 115866
 325    1.98  6.58   2.55  0.95   1.03           0.18           0.78
 326    0.06  0.22   0.08  0.03   0.03           0.01           1.02

 199       1.12     DIPHENYLMERCURY 587859
  77    0.53  1.75   0.68  0.26   0.26           0.05           2.94
 356    0.69  2.28   0.88  0.34   0.35           0.06           0.10

 200       0.94     TETRAPHENYLTIN
 197    1.10  3.66   1.57  0.61   0.44           0.11           1.56
 351    1.03  3.40   1.46  0.57   0.41           0.11           1.54

 201       0.63     BENZYLCHLORIDE 100447
  91    1.10  3.81   1.64  0.64   0.50           0.12           1.71
 126    0.30  1.03   0.45  0.17   0.12           0.03           0.47
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                Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56      Std #57      Std #58
Mass     109   236    136    -      82   128     98   116     84   112


 202       0.79     4-CHLOROBENZONITRILE 623030
 102     0.55  0.42   0.10         0.63  0.99   0.33  0.55   1.57  1.16
 137     2.10  1.57   0.36         2.38  3.79   1.25  2.08   5.95  4.40

 203       0.78     3-CHLOROBENZALDEHYDE 587042
 111     0.06  0.05   0.01         0.08  0.12   0.04  0.07   0.20  0.14
 139     0.12  0.10   0.02         0.15  0.24   0.08  0.13   0.38  0.28

 204       0.78     O-CHLOROANISOLE 766518
 127     0.60  0.46   0.11         0.69  1.09   0.36  0.60   1.71  1.27
 142     1.32  1.00   0.24         0.50  2.40   0.79  1.31   3.76  2.78

 205       0.01     CHLOROBENZAMIDE  619567
 139     0.70  0.55   0.13         0.77  1.25   0.50  0.84   1.57  1.16
 155     0.38  0.30   0.07         0.42  0.68   0.27  0.46   0.85  0.63

 206       0.78     3,4-DICHLOROBENZALDEHYDE 6287383
 173     0.48  0.39   0.09         0.58  0.93   0.31  0.57   1.46  1.07
 174     0.32  0.26   0.06         0.39  0.62   0.21  0.34   0.98  0.72

 207       0.73     1,2,4-TRICHLOROBENZENE 120821
 145     0.34  0.26   0.06         0.40  0.63   0.22  0.36   0.80  0.57
 180     1.30  1.00   0.24         1.50  2.40   0.83  1.37   3.03  2.16

 208       0.01     2-BROMO-1-CHLOROBENZENE 694804
 190     0.78  0.61   0.14         0.85  1.38   0.55  0.92   1.74  1.28
 192     1.04  0.81   0.19         1.14  1.84   0.74  1.24   2.33  1.71

 209       0.77     1,2-DICHLORONAPHTHALENE 2050693
 161     0.44  0.34   0.08         0.50  0.78   0.28  0.46   1.01  0.72
 196     2.17  1.67   0.40         2.51  3.88   1.38  2.29   5.03  3.58

 210       0.69     1,2,4,5-TETRACHLOROBENZENE 95943
 214     1.18  0.90   0.22         1.29  2.09   0.84  1.40   2.63  1.94
 216     1.54  1.18   0.28         1.69  2.72   1.09  1.83   3.43  2.52

 211       0.80     P-DIBROMOBENZENE 106376
 234     0.68  0.52   0.12         0.77  1.23   0.41  0.67   1.93  1.43
 236     1.29  1.00   0.23         1.48  2.36   0.78  1.30   3.77  2.93

 212       0.80     4-BROMODIPHENYLETHER
 248     1.08  0.81   0.20         1.19  1.92   0.77  1.29   2.42  1.78
 250     1.13  0.88   0.21         1.26  2.04   0.82  1.37   2.57  1.89

 213       0.01     HEXACHLOROBENZENE 118741
 284     0.74  0.56   0.13         0.84  1.34   0.44  0.73   2.10  1.55
 286     0.60  0.46   0.11         0.68  1.08   0.36  0.59   1.70  1.26

 214       0.58     PYRIDINE 110861
  52     0.29  0.22   0.05         0.33  0.51   0.19  0.32   0.67  0.48
  79     0.44  0.34   0.08         0.51  0.78   0.30  0.50   1.10  0.78
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              Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery    Compound Name
          Std #59       Std #60       Std #61        Std #62        Std #63
Mass      110   125     82   110     264    -       188    -        99    -


 202       0.79      4-CHLOROBENZONITRILE 623030
 102    0.39  1.35    0.58  0.23    0.18            0.04            0.61
 137    1.49  5.12    2.21  0.85    0.67            0.16            2.32

 203       0.78      3-CHLOROBENZALDEHYDE 587042
 111    0.05  0.17    0.07  0.03    0.02            0.00            0.08
 139    0.10  0.32    0.14  0.05    0.04            0.01            0.15

 204       0.78      O-CHLOROANISOLE 766518
 127    0.43  1.48    0.64  0.25    0.17            0.05            0.67
 142    0.94  3.24    1.40  0.54    0.36            0.10            1.46

 205       0.01      CHLOROBENZAMIDE  619567
 139    0.51  1.70    0.66  0.26    0.27            0.05            0.76
 155    0.28  0.92    0.36  0.14    0.15            0.03            0.41

 206       0.78      3,4-DICHLOROBENZALDEHYDE 6287383
 173    0.37  1.25    0.54  0.21    0.17            0.04            0.57
 174    0.25  0.84    0.36  0.14    0.11            0.03            0.38

 207       0.73      1,2,4-TRICHLOROBENZENE 120821
 145    0.24  0.80    0.33  0.13    0.12            0.03            0.36
 180    0.89  3.05    1.25  0.48    0.46            0.10            1.36

 208       0.01      2-BROMO-1-CHLOROBENZENE 694804
 190    0.57  1.88    0.73  0.28    0.30            0.05            0.84
 192    0.76  2.52    0.98  0.38    0.40            0.07            1.12

 209       0.77      1,2-DICHLORONAPHTHALENE 2050693
 161    0.31  1.02    0.42  0.16    0.15            0.03            0.46
 196    1.52  5.08    2.08  0.80    0.76            0.17            2.27

 210       0.69      1,2,4,5-TETRACHLOROBENZENE 95943
 214    0.86  2.85    1.11  0.43    0.45            0.08            1.27
 216    1.12  3.72    1.44  0.56    0.58            0.11            1.66

 211       0.80      P-DIBROMOBENZENE 106376
 234    0.49  1.66    0.72  0.28    0.19            0.05            0.75
 236    0.93  3.18    1.38  0.53    0.45            0.10            1.45

 212       0.80      4-BROMODIPHENYLETHER
 248    0.79  2.61    1.01  0.39    0.41            0.07            1.17
 250    0.84  2.78    1.08  0.42    0.44            0.08            1.24

 213       0.01      HEXACHLOROBENZENE 118741
 284    0.53  1.83    0.78  0.30    0.24            0.06            0.82
 286    0.43  1.46    0.63  0.24    0.19            0.05            0.66

 214       0.58      PYRIDINE 110861
  52    0.20  0.68    0.28  0.11    0.10            0.02            0.30
  79    0.33  1.11    0.42  0.16    0.17            0.04            0.50
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             Internal/External Standard File for Cmpd Class # 3

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54         Std #56        Std #57        Std #58
Mass     109   236    136    -         82   128       98   116       84   112


  215       0.66      ALPHA-PICOLINE 109068
  66     0.26  0.20    0.05           0.30  0.46     0.16  0.27     0.59  0.42
  93     0.66  0.51    0.12           0.76  1.18     0.40  0.66     1.52  1.09

  216       0.84      ANILINE 62533
  66     0.23  0.19    0.04           0.28  0.41     0.15  0.24     0.53  0.38
  93     0.76  0.54    0.13           0.81  1.25     0.45  0.74     1.62  1.15

  217       0.57      LUTIDINE  108485
 106     0.13  0.10    0.02           0.15  0.25     0.08  0.13     0.39  0.28
 107     0.22  0.16    0.04           0.24  0.39     0.13  0.21     0.61  0.45

  218       0.01      TOLUIDINE 106490
 106     0.89  0.69    0.16           0.97  1.57     0.64  1.07     1.97  1.45
 107     0.71  0.56    0.13           0.78  1.27     0.51  0.86     1.58  1.16

  219       0.86      INDOLE 120729
  90     0.72  0.54    0.13           0.82  1.30     0.43  0.71     2.04  1.51
 117     1.92  1.45    0.34           2.17  3.46     1.14  1.89     5.43  4.02

  220       0.82      2,3,6-TRIMETHYLPYRIDINE 1462846
 120     0.66  0.51    0.12           0.76  1.18     0.42  0.69     1.53  1.09
 121     0.90  0.69    0.17           1.03  1.61     0.55  0.91     2.08  1.49

  221       0.72      2,6-DIMETHYLANILINE 1300738
 106     0.36  0.27    0.06           0.41  0.65     0.21  0.36     1.02  0.75
 121     0.57  0.44    0.10           0.66  1.04     0.34  0.57     1.64  1.21

  222       0.88      M-CHLOROANILINE 108429
 127     1.09  0.84    0.20           1.26  1.94     0.69  1.15     2.52  1.79
 129     0.34  0.26    0.06           0.29  0.60     0.22  0.36     0.78  0.56

  223       0.77      QUINOLINE 91225
 129     1.82  1.41    0.34           1.99  3.22     1.30  2.17     4.06  2.98
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            Internal/External Standard File for Cmpd Class # 3

Cmpd#     Recovery   Compound Name
           Std #59      Std #60       Std #61        Std #62        Std #63
Mass      110   125    82    110    264     -      188     -      99     -


 215        0.66     ALPHA-PICOLINE 109068
 66      0.18  0.60   0.25  0.09   0.09           0.02           0.27
 93      0.46  1.54   0.63  0.24   0.23           0.05           0.69

 216        0.84     ANILINE 62533
 66      0.17  0.56   0.22  0.09   0.08           0.02           0.24
 93      0.49  1.64   0.67  0.26   0.24           0.05           0.73

 217        0.57     LUTIDINE  108485
106      0.10  0.33   0.14  0.05   0.04           0.01           0.15
107      0.16  0.52   0.23  0.09   0.06           0.02           0.24

 218        0.01     TOLUIDINE 106490
106      0.65  2.15   0.83  0.32   0.32           0.06           0.96
107      0.52  1.73   0.67  0.26   0.26           0.05           0.77

 219        0.86     INDOLE 120729
 90      0.51  1.75   0.76  0.29   0.23           0.05           0.79
117      1.40  4.68   2.02  0.78   0.61           0.15           2.12

 220        0.82     2,3,6-TRIMETHYLPYRIDINE 1462846
120      0.46  1.54   0.63  0.24   0.23           0.05           0.67
121      0.62  2.10   0.86  0.33   0.32           0.07           0.94

 221        0.72     2,6-DIMETHYLANILINE 1300738
106      0.26  0.88   0.38  0.15   0.11           0.03           0.40
121      0.42  1.41   0.61  0.24   0.18           0.04           0.64

 222        0.88     M-CHLOROANILINE 108429
127      0.76  2.55   1.05  0.40   0.38           0.98           1.14
129      0.24  0.79   0.33  0.13   0.12           0.03           0.35

 223        0.77     QUINOLINE 91225
129      1.33  4.40   1.70  0.66   0.69           0.12           1.96
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Table B-4. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NO. 1)

Class No. 4

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	NA	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	0.46	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	0.46	1.03(a)	.60(0)	-	.18(6)	1.07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	NA	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	NA	.97(4)	.57(10)	.95(10)	.16(3)	-	1.60(1)	2.35(17)	1.70(16)
	128	NA	.61(2)	.35(9)	.59(9)	.10(1)	.63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	84	NA	.42(15)	.25(24)	.42(24)	.071 ~~.11~~(18)	.44(16)	.70(15)	-	.73(2)
	112	NA	.58(15)	.35(22)	.58(23)	.098(18)	.61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	NA	1.09(4)	.65(13)	1.07(14)	.18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	NA	2.85(5)	1.67(13)	2.78(14)	.48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	NA	1.52(2)	.90(7)	1.50(8)	.25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	NA	.46(2)	.27(8)	.45(7)	~~.16~~(3) .076	.48(3)	.76(4)	1.11(18)	.81(17)
d_{12}-perylene	264	NA	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	NA	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	NA	1.10(4)	.65(7)	1.08(8)	.18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	NA	1.43(4)	.84(6)	1.39(7)	.24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(continued)

			Standard							
			d_5-Propiophenone		d_5-Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-iodotoluene	
Compound	Ion	Recovery	m/z 82	m/z 110	m/z 110	m/z 125	m/z 264	m/z 188	m/z 109	m/z 236
d_5-phenol	99	NA	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-*o*-xylene	98	0.46	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	0.46	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	NA	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	NA	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	NA	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	NA	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	NA	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	NA	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	NA	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	NA	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	NA	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	NA	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	NA	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

[a] (CV).

```
          Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56       Std #57       Std #58
Mass     109   236    136    -       82   128      98   116      84   112


 100       0.51     N-TRIDECANE 629505
  43    2.18  1.64   0.34          2.48  3.95    1.30  2.16    6.20  4.58
  57    2.75  2.09   0.50          3.14  5.01    1.66  2.77    7.93  5.86

 101       0.45     N-TETRADECANE 629594
  43    2.52  1.92   0.45          2.88  4.58    1.51  2.51    7.19  5.31
  57    3.40  2.55   0.61          3.87  6.16    2.03  3.37    9.67  7.15

 102       0.62     N-PENTADECANE 692629
  57    2.78  2.14   0.52          3.22  4.99    1.77  2.94    6.47  4.62
  71    1.73  1.33   0.32          2.01  3.11    1.10  1.83    4.03  2.87

 103       0.51     N-HEXADECANE 544763
  43    1.90  1.45   0.34          2.16  3.45    1.13  1.89    5.41  3.99
  57    2.72  2.08   0.49          3.11  4.96    1.63  2.71    7.78  5.74

 104       0.77     N-HEPTADECANE 629787
  57    3.13  2.41   0.58          3.61  5.59    1.99  3.30    7.25  5.17
  71    2.07  1.60   0.38          2.39  3.70    1.32  2.18    4.80  3.42

 105       0.66     N-OCTADECANE 593453
  57    2.99  2.51   0.59          3.75  5.98    1.88  3.14    8.96  6.63
  71    1.98  1.66   0.39          2.48  3.95    1.25  2.08    5.95  4.41

 106       0.65     N-NONADECANE 629925
  71    2.12  1.61   0.38          2.42  3.85    1.27  2.11    6.04  4.47
  85    1.42  1.08   0.25          1.61  2.57    0.85  1.41    4.03  2.98

 107       0.82     N-EICOSANE 1112958
  57    4.43  3.41   0.82          5.11  7.92    2.82  4.66   10.26  7.32
  71    3.03  2.33   0.56          3.50  5.43    1.93  3.19    7.03  5.01

 108       0.65     N-HENEICOSANE 629947
  57    3.93  2.96   0.70          4.43  7.05    2.32  3.86   11.05  8.20
  71    2.71  2.05   0.48          3.07  4.88    1.61  2.67    7.65  5.68

 109       0.59     N-DOCOSANE 629970
  57    3.73  2.98   0.70          4.46  7.10    2.33  3.88   11.11  8.26
  71    2.60  2.08   0.49          3.11  4.96    1.63  2.70    7.76  5.77

 110       0.58     N-TRICOSANE 638675
  57    3.99  3.19   0.75          4.77  7.60    2.49  4.14   11.85  8.83
  71    2.80  2.24   0.53          3.35  5.34    1.75  2.91    8.33  6.20

 111       0.48     2-METHYLNAPHTHALENE 91576
 141    2.03  1.58   0.38          2.23  3.60    1.44  2.42    4.53  3.34
 142    2.51  1.96   0.46          2.76  4.45    1.79  2.99    5.62  4.13

 112       0.50     ACENAPHTHENE 83329
 153    1.26  0.98   0.23          1.38  2.22    0.89  1.49    2.81  2.06
 154    3.40  2.64   0.63          3.73  6.02    2.41  4.04    7.59  5.58
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           Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std #59     Std #60       Std #61        Std #62        Std #63
Mass      110   125    82   110     264     -      188     -       99     -


 100       0.51     N-TRIDECANE 629505
  43     1.56  5.33   2.30  0.89    0.70           0.17           2.41
  57     1.99  6.75   2.94  1.14    0.76           0.21           3.09

 101       0.45     N-TETRADECANE 629594
  43     1.86  6.19   2.67  1.03    0.80           0.19           2.80
  57     2.50  8.33   3.57  1.39    1.08           0.26           3.77

 102       0.62     N-PENTADECANE 692629
  57     1.94  6.52   2.68  1.03    0.99           0.22           2.92
  71     1.21  4.06   1.67  0.64    0.62           0.14           1.82

 103       0.51     N-HEXADECANE 544763
  43     1.40  4.66   2.01  0.78    0.61           0.15           2.11
  57     2.01  6.70   2.88  1.12    0.87           0.21           3.03

 104       0.77     N-HEPTADECANE 629787
  57     2.18  7.32   3.01  1.16    1.11           0.24           3.27
  71     1.44  4.85   1.99  0.77    0.73           0.16           2.17

 105       0.66     N-OCTADECANE 593453
  57     2.33  8.10   3.48  1.35    1.01           0.24           3.65
  71     1.55  5.35   2.30  0.89    0.58           0.06           2.41

 106       0.65     N-NONADECANE 629925
  71     1.51  5.27   2.24  0.87    0.68           0.16           2.35
  85     1.01  3.47   1.50  0.58    0.45           0.11           1.57

 107       0.82     N-EICOSANE 1112958
  57     3.08 10.35   4.25  1.63    1.57           0.35           4.63
  71     2.11  7.09   2.91  1.12    1.07           0.23           3.17

 108       0.65     N-HENEICOSANE 629947
  57     2.73  9.53   4.11  1.60    1.07           0.30           4.31
  71     1.89  6.60   2.85  1.10    0.74           0.21           2.99

 109       0.59     N-DOCOSANE 629970
  57     2.89  9.60   4.14  1.60    1.22           0.30           4.35
  71     2.02  6.71   2.89  1.12    0.85           0.21           3.04

 110       0.58     N-TRICOSANE 638675
  57     3.10 10.28   4.42  1.71    1.29           0.32           4.65
  71     2.18  7.22   3.11  1.20    0.90           0.22           3.27

 111       0.48     2-METHYLNAPHTHALENE 91576
 141     1.48  4.91   1.90  0.74    0.77           0.14           2.19
 142     1.78  6.08   2.36  0.91    0.95           0.17           2.71

 112       0.50     ACENAPHTHENE 83329
 153     0.92  3.04   1.18  0.46    0.47           0.09           1.35
 154     2.48  8.22   3.19  1.23    1.28           0.23           3.66
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           Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56      Std #57      Std #58
Mass     109   236    136    -       82   128     98   116     84   112


 113       0.01     BIPHENYL 92524
154    2.28  1.78    0.42           2.51  4.04   1.63  2.72   5.10  3.75

 114       0.48     1,8-DIMETHYLNAPHTHALENE 569415
141    1.59  1.24    0.29           1.74  2.82   1.13  1.89   3.55  2.61
156    2.30  1.79    0.42           2.52  4.07   1.63  2.73   5.13  3.77

 115       0.57     DI-T-BUTYLDISULFIDE 110065
 41    0.73  0.56    0.13           0.84  1.34   0.44  0.73   2.10  1.55
 57    3.09  2.36    0.56           3.54  5.64   1.85  3.09   8.84  6.54

 116       0.96     ALDRIN  309002
 66    1.33  1.03    0.24           1.49  2.40   0.97  1.62   3.03  2.23
263    0.60  0.46    0.11           0.67  1.08   0.44  0.73   1.36  1.00

 117       0.01     PYRIDINE 110861
 52    0.29  0.22    0.05           0.33  0.51   0.19  0.32   0.67  0.48
 79    0.44  0.34    0.08           0.51  0.78   0.30  0.50   1.10  0.78

 118       0.01     ALPHA-PICOLINE 109068
 66    0.26  0.20    0.05           0.30  0.46   0.16  0.27   0.59  0.42
 93    0.66  0.51    0.12           0.76  1.18   0.40  0.66   1.52  1.09

 119       0.01     ANILINE 62533
 66    0.23  0.19    0.04           0.28  0.41   0.15  0.24   0.53  0.38
 93    0.76  0.54    0.13           0.81  1.25   0.45  0.74   1.62  1.15

 120       0.01     LUTIDINE 108485
106    0.13  0.10    0.02           0.15  0.25   0.08  0.13   0.39  0.28
107    0.22  0.16    0.04           0.24  0.39   0.13  0.21   0.61  0.45

 121       0.01     TOLUIDINE  106490
106    0.89  0.69    0.16           0.97  1.57   0.64  1.07   1.97  1.45
107    0.71  0.56    0.13           0.78  1.27   0.51  0.86   1.58  1.16

 122       0.01     INDOLE 120729
 90    0.72  0.54    0.13           0.82  1.30   0.43  0.71   2.04  1.51
117    1.92  1.45    0.34           2.17  3.46   1.14  1.89   5.43  4.02

 123       0.01     2,3,6-TRIMETHYLPYRIDINE 1462846
120    0.66  0.51    0.12           0.76  1.18   0.42  0.69   1.53  1.09
121    0.90  0.69    0.17           1.03  1.61   0.55  0.91   2.08  1.49

 124       0.01     2,6-DIMETHYLANILINE 1300738
106    0.36  0.27    0.06           0.41  0.65   0.21  0.36   1.02  0.75
121    0.57  0.44    0.10           0.66  1.04   0.34  0.57   1.64  1.21

 125       0.01     M-CHLOROANILINE 108429
127    1.09  0.84    0.20           1.26  1.94   0.69  1.15   2.52  1.79
129    0.34  0.26    0.06           0.29  0.60   0.22  0.36   0.78  0.56
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           Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery    Compound Name
           Std #59       Std #60        Std #61        Std #62        Std #63
Mass     110   125       82   110       264    -       188    -        99    -


 113       0.01      BIPHENYL 92524
 154    1.67  5.52    2.14  0.83     0.87           0.16           2.46

 114       0.48      1,8-DIMETHYLNAPHTHALENE 569415
 141    1.16  3.84    1.49  0.58     0.60           0.11           1.71
 156    1.67  5.55    2.15  0.83     0.87           0.16           2.48

 115       0.57      DI-T-BUTYLDISULFIDE 110065
  41    0.54  1.78    0.78  0.31     0.20           0.06           0.82
  57    2.21  7.62    3.29  1.27     1.00           0.24           3.42

 116       0.96      ALDRIN  309002
  66    0.99  3.28    1.27  0.49     0.51           0.09           1.46
 263    0.44  1.47    0.57  0.22     0.23           0.04           0.66

 117       0.01      PYRIDINE 110861
  52    0.20  0.68    0.28  0.11     0.10           0.02           0.30
  79    0.33  1.11    0.42  0.16     0.17           0.04           0.50

 118       0.01      ALPHA-PICOLINE 109068
  66    0.18  0.60    0.25  0.09     0.09           0.02           0.27
  93    0.46  1.54    0.63  0.24     0.23           0.05           0.69

 119       0.01      ANILINE 62533
  66    0.17  0.56    0.22  0.09     0.08           0.02           0.24
  93    0.49  1.64    0.67  0.26     0.24           0.05           0.73

 120       0.01      LUTIDINE 108485
 106    0.10  0.33    0.14  0.05     0.04           0.01           0.15
 107    0.16  0.52    0.23  0.09     0.06           0.02           0.24

 121       0.01      TOLUIDINE  106490
 106    0.65  2.15    0.83  0.32     0.32           0.06           0.96
 107    0.52  1.73    0.67  0.26     0.26           0.05           0.77

 122       0.01      INDOLE 120729
  90    0.51  1.75    0.76  0.29     0.23           0.05           0.79
 117    1.40  4.68    2.02  0.78     0.61           0.15           2.12

 123       0.01      2,3,6-TRIMETHYLPYRIDINE 1462846
 120    0.46  1.54    0.63  0.24     0.23           0.05           0.67
 121    0.62  2.10    0.86  0.33     0.32           0.07           0.94

 124       0.01      2,6-DIMETHYLANILINE 1300738
 106    0.26  0.88    0.38  0.15     0.11           0.03           0.40
 121    0.42  1.41    0.61  0.24     0.18           0.04           0.64

 125       0.01      M-CHLOROANILINE 108429
 127    0.76  2.55    1.05  0.40     0.38           0.98           1.14
 129    0.24  0.79    0.33  0.13     0.12           0.03           0.35
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            Internal/External Standard File for Cmpd Class # 4

   Cmpd#    Recovery    Compound Name
              Std # 2     Std #54         Std #56        Std #57         Std #58
   Mass     109   236     136     -       82    128      98    116       84    112


    126       0.01      QUINOLINE 91225
    129    1.82  1.41     0.34            1.99  3.22     1.30  2.17     4.06  2.98

    127       0.01      P-NITROANILINE 100016
     65    0.44  0.35     0.08            0.52  0.83     0.27  0.46     1.30  0.97
    138    0.56  0.45     0.11            0.67  1.07     0.35  0.58     1.68  0.22

    128       0.01      2,4-DIMETHYLQUINOLINE 1198374
    156    0.41  0.32     0.08            0.47  0.75     0.26  0.43     0.95  0.68
    157    2.01  1.54     0.37            2.31  3.59     1.27  2.11     4.64  3.31

    129       0.01      1,8-DIAMINONAPHTHALENE 569415
    114    0.03  0.02     0.00            0.04  0.06     0.02  0.03     0.09  0.06
    141    0.05  0.04     0.01            0.06  0.01     0.03  0.05     0.14  0.11

    130       0.01      NICOTINE 54115
     84    1.17  0.90     0.22            1.35  2.09     0.74  1.23     2.70  1.92
    133    0.28  0.21     0.05            0.32  0.49     0.17  0.29     0.63  0.45

    131       0.01      CARBAZOLE 86748
    167    3.73  2.88     0.69            4.30  6.66     2.37  3.92     9.36  6.67

    132       0.01      2-AMINOBIPHENYL 90445
    168    6.79  5.11     1.20            7.65 12.18     4.61  6.67    19.13 14.17
    169   12.72  9.45     2.22           14.15 22.54     7.42 12.30    35.40 26.19

    133       0.01      DIPHENYLAMINE 122394
    168    1.48  1.14     0.27            1.71  2.65     0.94  1.56     3.43  2.45
    169    2.79  2.15     0.52            3.22  4.99     1.77  2.93     6.45  4.60

    134       0.01      DICYCLOHEXYLAMINE 122394
     56    0.33  0.37     0.06            0.39  0.63     0.21  0.35     1.10  0.78
    138    0.96  0.76     0.18            1.12  1.80     0.61  1.02     3.15  2.25

    135       0.01      TRIBUTYLAMINE 102829
    100    0.42  0.33     0.08            0.49  0.75     0.27  0.44     0.97  0.69
    142    1.53  1.18     0.28            1.77  2.74     0.97  1.61     3.52  2.51

    136       0.01      CAFFEINE 58082
    109    0.10  0.08     0.02            0.12  0.17     0.06  0.10     0.23  0.16
    194    0.19  0.15     0.04            0.22  0.34     0.12  0.20     0.44  0.32

    137       0.01      DIBENZYLAMINE 103491
     91    1.62  1.26     0.30            1.78  2.87     1.16  1.94     3.63  2.67
    197    0.13  0.11     0.03            0.15  0.24     0.10  0.16     0.30  0.22

    138       0.01      N,N-DIMETHYLDODECYLAMINE 112185
     58    4.72  3.88     0.87            5.47  8.83     3.58  5.99    11.09  8.16
     59    0.17  0.13     0.03            0.20  0.30     0.13  0.21     0.40  0.29

    139       0.01      ATRAZINE 1912249
    200    2.75  2.20     0.52            3.28  5.23     1.72  2.86     8.17  6.09
    215    1.67  1.34     0.31            2.00  3.18     1.05  1.74     4.97  3.71
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                Internal/External Standard File for Cmpd Class # 4

Cmpd#     Recovery     Compound Name
           Std #59       Std #60       Std #61        Std #62        Std #63
Mass      110    125     82    110     264     -      188     -       99     -


 126        0.01       QUINOLINE 91225
 129     1.33   4.40    1.70  0.66    0.69            0.12            1.96

 127        0.01       P-NITROANILINE 100016
  65     0.34   1.13    0.49  0.19    0.14            0.04            0.51
 138     0.43   1.84    0.62  0.24    0.19            0.05            0.65

 128        0.01       2,4-DIMETHYLQUINOLINE 1198374
 156     0.29   0.96    0.40  0.15    0.15            0.03            0.43
 157     1.46   4.69    1.93  0.74    0.71            0.15            2.09

 129        0.01       1,8-DIAMINONAPHTHALENE 569415
 114     0.02   0.08    0.03  0.01    0.01            0.00            0.03
 141     0.04   0.12    0.05  0.02    0.01            0.00            0.55

 130        0.01       NICOTINE 54115
  84     0.82   2.74    1.12  0.43    0.41            0.09            1.22
 133     0.19   0.64    0.26  0.10    0.10            0.02            0.29

 131        0.01       CARBAZOLE 86748
 167     2.60   8.72    3.57  1.37    1.28            0.31            4.22

 132        0.01       2-AMINOBIPHENYL 90445
 168     4.75  16.46    7.10  2.75    2.13            0.51            7.45
 169     8.82  30.44   13.14  5.08    3.96            0.95           13.80

 133        0.01       DIPHENYLAMINE 122394
 168     1.03   3.47    1.42  0.55    0.52            0.11            1.55
 169     1.94   6.46    2.68  1.03    0.98            0.22            2.91

 134        0.01       DICYCLOHEXYLAMINE 122394
  56     0.25   0.81    0.33  0.14    0.09            0.03            0.38
 138     0.71   2.34    0.95  0.40    0.26            0.08            1.09

 135        0.01       TRIBUTYLAMINE 102829
 100     0.29   0.99    0.41  0.16    0.15            0.03            0.44
 142     0.99   3.34    1.47  0.57    0.53            0.12            1.59

 136        0.01       CAFFEINE 58082
 109     0.07   0.23    0.09  0.04    0.04            0.01            0.10
 194     0.13   0.45    0.18  0.07    0.07            0.02            0.21

 137        0.01       DIBENZYLAMINE 103491
  91     1.18   3.91    1.52  0.59    0.62            0.11            1.74
 197     0.10   0.32    0.13  0.05    0.05            0.01            0.14

 138        0.01       N,N-DIMETHYLDODECYLAMINE 112185
  58     3.62  12.02    4.66  1.81    1.87            0.34            5.37
  59     0.13   0.43    0.17  0.06    0.07            0.01            0.19

 139        0.01       ATRAZINE 1912249
 200     2.13   7.07    3.05  1.18    0.90            0.22            3.26
 215     1.21   4.30    1.85  0.72    0.55            0.13            1.95
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          Internal/External Standard File for Cmpd Class # 4

 Cmpd#   Recovery   Compound Name
          Std # 2     Std #54        Std #56      Std #57      Std #58
 Mass     109  236    136    -        82  128      98  116      84  112


  140      0.01     HEPTANONE(2)  110430
   43    1.21  0.94   0.22          1.33  2.14   0.85  1.14   2.32  2.00
   58    0.75  0.58   0.14          0.83  1.33   0.53  0.88   1.69  1.25

  141      0.01     BUTOXYETHANOL  111762
   41    0.21  0.17   0.04          0.25  0.40   0.13  0.22   0.49  0.35
   57    0.55  0.42   0.10          0.63  1.03   0.35  0.58   1.27  0.91

  142      0.01     2-OCTANONE  111137
   43    1.30  1.01   0.24          1.43  2.31   0.91  1.53   2.92  2.15
   58    1.02  0.79   0.19          1.11  1.80   0.71  1.19   2.27  1.67

  143      0.01     BUTYLPROPIONATE  590012
   57    1.48  1.14   0.27          1.71  2.73   0.90  1.49   4.27  3.15
   75    0.44  0.34   0.08          0.51  0.82   0.27  0.45   1.28  0.95

  144      0.01     ISOPHORONE  78591
   82    1.77  1.36   0.33          2.04  3.17   1.13  1.86   4.11  2.93
  138    0.39  0.30   0.07          0.45  0.72   0.25  0.41   0.90  0.64

  145      0.01     FENCHONE  1195759
   69    0.66  0.51   0.12          0.72  1.17   0.47  0.78   1.47  1.08
   81    1.44  1.12   0.27          1.58  2.55   1.02  1.71   3.22  2.36

  146      0.01     ALPHA-TERPINEOL  98555
   59    0.56  0.43   0.10          0.65  1.00   0.36  0.59   1.31  0.93
  136    0.32  0.25   0.06          0.37  0.58   0.21  0.34   0.75  0.53

  147      0.01     N-DECANOL  112301
   41    0.40  0.31   0.07          0.46  0.74   0.25  0.42   0.92  0.66
   43    0.44  0.34   0.08          0.51  0.79   0.28  0.46   1.02  0.73

  148      0.01     DIMETHYLADIPATE   627930
   59    0.56  0.45   0.10          0.64  1.03   0.41  0.69   1.29  0.95
  114    0.44  0.35   0.08          0.49  0.79   0.32  0.54   1.00  0.74

  149      0.01     METHYLSTEARATE  112618
   74    3.42  2.65   0.63          3.89  6.28   2.54  4.25   7.90  5.81
   87    2.22  1.72   0.41          2.52  4.07   1.65  2.76   5.13  3.77

  150      0.01     N-DECANE
   43    1.47  1.11   0.26          1.67  2.66   0.88  1.46   4.18  3.09
   57    1.42  1.08   0.25          1.64  2.61   0.85  1.41   4.05  3.00

  151      0.01     PHENYLACETATE  122792
   94    1.84  1.43   0.34          2.01  3.25   1.30  2.18   4.10  3.01
  136    0.25  0.20   0.05          0.28  0.45   0.18  0.30   0.57  0.42

  152      0.01     BENZYLACETATE  140114
   91    0.52  0.40   0.09          0.57  0.92   0.37  0.62   1.15  0.85
  108    1.09  0.85   0.20          1.19  1.92   0.77  1.29   2.43  1.79
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            Internal/External Standard File for Cmpd Class # 4

   Cmpd#    Recovery    Compound Name
             Std #59       Std #60       Std #61        Std #62        Std #63
   Mass     110   125     82    110     264     -      188     -       99     -


    140       0.01      HEPTANONE(2)  110430
     43     0.88  2.91   1.13  0.44    0.47            0.08            1.30
     58     0.55  1.82   0.71  0.27    0.29            0.05            0.81

    141       0.01      BUTOXYETHANOL  111762
     41     0.15  0.49   0.20  0.09    0.07            0.02            0.22
     57     0.38  1.28   0.52  0.20    0.19            0.04            0.57

    142       0.01      2-OCTANONE  111137
     43     0.95  3.14   1.22  0.47    0.51            0.09            1.40
     58     0.74  2.45   0.95  0.37    0.39            0.07            1.09

    143       0.01      BUTYLPROPIONATE  590012
     57     1.11  3.69   1.59  0.61    0.48            0.12            1.66
     75     0.33  1.11   0.48  0.19    0.15            0.04            0.50

    144       0.01      ISOPHORONE  78591
     82     1.23  4.14   1.70  0.65    0.62            0.14            1.80
    138     0.27  0.91   0.37  0.14    0.14            0.03            0.41

    145       0.01      FENCHONE  1195759
     69     0.48  1.58   0.62  0.24    0.25            0.05            0.71
     81     1.05  3.45   1.35  0.52    0.55            0.10            1.55

    146       0.01      ALPHA-TERPINEOL  98555
     59     0.39  1.31   0.54  0.21    0.20            0.04            0.58
    136     0.23  0.76   0.31  0.12    0.11            0.03            0.34

    147       0.01      N-DECANOL  112301
     41     0.28  0.93   0.38  0.15    0.14            0.03            0.41
     43     0.31  1.63   0.42  0.16    0.15            0.03            0.46

    148       0.01      DIMETHYLADIPATE   627930
     59     0.42  1.40   0.54  0.21    0.22            0.04            0.62
    114     0.33  1.08   0.42  0.16    0.17            0.03            0.48

    149       0.01      METHYLSTEARATE  112618
     74     2.58  8.56   3.32  1.29    1.33            0.24            3.83
     87     1.67  5.55   2.15  0.83    0.87            0.16            2.48

    150       0.01      N-DECANE
     43     1.05  3.59   1.55  0.60    0.47            0.11            1.62
     57     1.01  3.48   1.50  0.58    0.46            0.11            1.58

    151       0.01      PHENYLACETATE  122792
     94     1.31  4.43   1.72  0.67    0.70            0.13            1.98
    136     0.18  0.62   0.24  0.09    0.10            0.02            0.28

    152       0.01      BENZYLACETATE  140114
     91     0.38  1.25   0.48  0.19    0.20            0.04            0.56
    108     0.79  2.63   1.02  0.40    0.41            0.07            1.17
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         Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass      109   236    136    -      82   128      98   116      84   112


  153      0.01      METHYLBENZENESULFONATE
   77    1.24  0.94   0.22         1.41  2.25    0.74  1.23    3.54  2.61
  172    0.44  0.34   0.08         0.50  0.80    0.26  0.44    1.26  0.93

  154      0.01      METHYLTOLUENESULFONATE(P)
   91    1.60  1.21   0.29         1.81  2.89    0.95  1.58    4.53  3.35
  155    0.72  0.54   0.13         0.81  1.29    0.42  0.71    2.02  1.50

  155      0.01      DIMETHYLPHTHALATE  131113
   77    0.81  0.63   0.15         0.94  1.45    0.52  0.85    1.88  1.34
  163    5.29  4.07   0.98         6.10  9.46    3.36  5.56   12.22  8.71

  156      0.01      ETHYLTOLUENESULFONATE(P) 80400
   91    1.74  1.32   0.31         1.97  3.14    1.03  1.72    4.92  3.65
  155    1.18  0.94   0.22         1.40  2.23    0.73  1.21    3.46  2.35

  157      0.01      DIETHYLPHTHALATE  84662
  149    3.19  2.43   0.57         3.65  5.79    1.90  3.17    9.08  6.71
  177    0.80  0.61   0.14         0.93  1.47    0.48  0.80    2.29  1.69

  158      0.01      DIBUTYLPHTHALATE  84742
   57    0.29  0.23   0.05         0.34  0.52    0.19  0.31    0.68  0.48
  149    7.17  5.52   1.33         8.27 12.80    4.55  7.54   16.55 11.80

  159      0.01      BUTYLBENZYLPHTHALATE
   91    2.09  1.62   0.38         2.28  3.69    1.48  2.48    4.64  3.41
  149    3.37  2.62   0.62         3.69  5.95    2.40  4.01    7.49  5.51

  160      0.01      DIETHYLHEXYLPHTHALATE  117817
  149    5.22  4.07   0.96         5.71  9.23    3.74  6.26   11.59  8.53
  167    1.98  1.54   0.37         2.17  3.51    1.42  2.37    4.40  3.24

  161      0.01      BENZALDEHYDE  100527
   77    0.36  0.28   0.07         0.42  0.64    0.23  0.38    0.84  0.60
  105    0.40  0.31   0.07         0.46  0.70    0.25  0.42    0.92  0.66

  162      0.01      TOLUALDEHYDE  529204
   91    0.54  0.44   0.10         0.65  1.04    0.34  0.57    1.65  1.21
  119    0.63  0.51   0.12         0.77  1.23    0.41  0.68    1.95  1.43

  163      0.01      ACETOPHENONE 98862
   77    0.38  0.64   0.15         0.96  1.53    0.53  0.87    1.93  1.37
  105    1.22  0.94   0.23         1.41  2.25    0.78  1.29    2.85  2.03

  164      0.01      SALICYLALDEHYDE  90028
  121    0.56  0.44   0.10         0.61  0.99    0.40  0.67    1.24  0.91
  122    0.60  0.47   0.11         0.60  1.07    0.43  0.72    1.34  0.99

  165      0.01      ANISALDHYDE  123115
  135    1.37  1.08   0.25         1.53  2.47    0.91  1.66    3.11  2.29
  136    0.96  0.76   0.18         1.07  1.73    0.70  1.16    2.18  1.60
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           Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery    Compound Name
          Std #59       Std #60        Std #61        Std #62        Std #63
Mass     110   125     82   110     264     -      188     -       99     -


 153      0.01       METHYLBENZENESULFONATE
  77    0.91  3.04    1.31  0.51    0.40            0.09           1.38
 172    0.32  1.08    0.47  0.18    0.14            0.03           0.49

 154      0.01       METHYLTOLUENESULFONATE(P)
  91    1.17  3.90    1.68  0.65    0.51            0.12           1.76
 155    0.52  1.74    0.75  0.29    0.23            0.05           0.79

 155      0.01       DIMETHYLPHTHALATE  131113
  77    0.57  1.83    0.75  0.29    0.28            0.06           0.85
 163    3.68 11.87    4.88  1.88    1.85            0.41           5.51

 156      0.01       ETHYLTOLUENESULFONATE(P) 80400
  91    1.28  4.25    1.83  0.71    0.55            0.13           1.92
 155    0.91  3.01    1.30  0.50    0.38            0.09           1.36

 157      0.01       DIETHYLPHTHALATE  84662
 149    2.35  7.82    3.34  1.30    1.02            0.24           3.54
 177    0.59  1.97    0.85  0.33    0.26            0.06           0.89

 158      0.01       DIBUTYLPHTHALATE  84742
  57    0.20  0.68    0.28  0.11    0.10            0.02           0.31
 149    4.99 16.75    6.88  2.64    2.52            0.55           7.47

 159      0.01       BUTYLBENZYLPHTHALATE
  91    1.51  5.02    1.95  0.76    0.78            0.14           2.24
 149    2.44  8.10    3.15  1.22    1.26            0.23           3.62

 160      0.01       DIETHYLHEXYLPHTHALATE  117817
 149    4.03 12.58    4.88  1.89    1.90            0.35           5.61
 167    1.53  4.78    1.85  0.72    0.72            0.13           2.13

 161      0.01       BENZALDEHYDE  100527
  77    0.25  0.84    0.35  0.13    0.13            0.03           0.38
 105    0.28  0.93    0.38  0.15    0.14            0.03           0.42

 162      0.01       TOLUALDEHYDE  529204
  91    0.42  1.41    0.61  0.24    0.15            0.05           0.64
 119    0.50  1.66    0.72  0.28    0.22            0.05           0.75

 163      0.01       ACETOPHENONE 98862
  77    0.57  1.95    0.80  0.31    0.29            0.06           0.87
 105    0.85  2.88    1.18  0.45    0.43            0.09           1.28

 164      0.01       SALICYLALDEHYDE  90028
 121    0.41  1.35    0.52  0.20    0.21            0.04           0.60
 122    0.44  1.46    0.56  0.22    0.23            0.04           0.65

 165      0.01       ANISALDHYDE  123115
 135    1.01  3.36    1.30  0.51    0.53            0.09           1.50
 136    0.71  2.36    0.91  0.35    0.37            0.07           1.05
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             Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass     109   236    136    -       82   128      98   116      84   112


 166        0.01     PHENOL 108952
  94     1.07  0.84   0.20          1.18  1.90    0.76  1.27    2.41  1.77

 167        0.01     CRESOL(P) 106445
 107     1.21  0.93   0.23          1.40  2.25    0.80  1.29    2.91  2.08
 108     1.07  0.82   0.20          1.24  1.99    0.69  1.14    2.58  1.84

 168        0.01     2,3-DIMETHYLPHENOL  526750
 107     0.87  0.67   0.16          1.00  1.61    0.57  0.95    2.08  1.48
 122     0.91  0.70   0.17          1.05  1.64    0.58  0.96    2.12  1.51

 169        0.01     ISOPROPYLPHENOL  88699
 121     1.79  1.36   0.32          2.04  3.25    1.07  1.78    5.10  3.77
 136     0.07  0.56   0.12          0.75  1.19    0.39  0.65    1.87  1.38

 170        0.01     O-NITROPHENOL  88755
  65     0.03  0.02   0.00          0.03  0.05    0.02  0.03    0.06  0.05
 139     0.13  0.10   0.02          0.14  0.23    0.09  0.15    0.29  0.21

 171        0.01     4-CHLORO-3-METHYLPHENOL 59507
 107     0.93  0.71   0.17          1.06  1.68    0.55  0.92    2.64  2.95
 142     1.02  0.77   0.18          1.16  1.84    0.61  1.01    2.89  2.14

 172        0.01     4-CHLOROCRESOL
 107     0.83  0.64   0.16          0.97  1.57    0.53  0.88    2.03  1.45
 142     0.94  0.72   0.17          1.09  1.77    0.60  0.99    2.29  1.63

 173        0.01     1-NAPHTHOL   90153
 115     0.35  0.26   0.06          0.38  0.61    0.20  0.34    0.96  0.72
 144     0.61  0.45   0.11          0.67  1.07    0.35  0.29    1.68  1.25

 174        0.01     P-TERT-BUTYLPHENOL 98544
 107     0.56  0.43   0.10          0.65  1.03    0.34  0.56    1.60  1.18
 135     1.96  1.49   0.35          2.22  3.54    1.17  1.94    5.56  4.11

 175        0.01     2-NITROCRESOL 119335
  77     0.26  0.20   0.05          0.30  0.46    0.07  0.27    0.60  0.43
 153     0.74  0.57   0.14          0.83  1.33    0.46  0.78    1.72  1.23

 176        0.01     2,4-DICHLOROPHENOL  120832
 162     1.13  0.88   0.21          1.24  2.00    0.80  1.34    2.52  1.86
 164     0.72  0.53   0.13          0.78  1.27    0.51  0.85    1.60  1.18

 177        0.01     2,4,6-TRICHLOROPHENOL   88062
 196     0.81  0.63   0.15          0.89  1.44    0.58  0.97    1.88  1.34
 198     0.83  0.64   0.15          0.91  1.46    0.59  0.98    1.90  1.36

 178        0.01     DI-TERT-BUTYL-4-METHYLPHENOL   128370
 205     2.53  1.97   0.47          2.78  4.49    1.81  3.03    5.66  4.16
 220     0.67  0.52   0.12          0.73  1.18    0.48  0.80    1.49  1.09
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              Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery    Compound Name
          Std #59       Std #60       Std #61         Std #62         Std #63
Mass     110   125     82   110      264     -       188     -        99     -


 166       0.01      PHENOL 108952
  94     0.75  2.60   1.01  0.39    0.41            0.07             1.15

 167       0.01      CRESOL(P) 106445
 107     0.88  2.85   1.17  0.45    0.44            0.10             1.31
 108     0.78  2.52   1.03  0.40    0.39            0.09             1.16

 168       0.01      2,3-DIMETHYLPHENOL  526750
 107     0.63  2.11   0.84  0.32    0.32            0.07             0.94
 122     0.64  2.14   0.85  0.33    0.32            0.07             0.95

 169       0.01      ISOPROPYLPHENOL  88699
 121     1.28  4.39   1.90  0.73    0.58            0.14             1.99
 136     0.47  1.61   0.69  0.27    0.21            0.05             0.73

 170       0.01      O-NITROPHENOL  88755
  65     0.02  0.07   0.03  0.01    0.01            0.00             0.03
 139     0.09  0.31   0.12  0.05    0.05            0.01             0.14

 171       0.01      4-CHLORO-3-METHYLPHENOL 59507
 107     0.66  2.27   0.98  0.38    0.30            0.07             1.03
 142     0.72  2.49   1.07  0.42    0.32            0.08             1.13

 172       0.01      4-CHLOROCRESOL
 107     0.58  1.96   0.80  0.31    0.31            0.07             0.91
 142     0.66  2.20   0.85  0.34    0.35            0.08             1.03

 173       0.01      1-NAPHTHOL   90153
 115     0.25  0.83   0.36  0.14    0.11            0.03             0.38
 144     0.44  1.45   0.62  0.24    0.18            0.05             0.66

 174       0.01      P-TERT-BUTYLPHENOL 98544
 107     0.40  1.38   0.66  0.23    0.18            0.04             0.62
 135     1.44  4.79   2.04  0.80    0.63            0.15             2.16

 175       0.01      2-NITROCRESOL 119335
  77     0.18  0.61   0.25  0.10    0.09            0.02             0.27
 153     0.52  1.74   0.71  0.27    0.26            0.06             0.78

 176       0.01      2,4-DICHLOROPHENOL  120832
 162     0.80  2.73   1.05  0.41    0.43            0.08             1.22
 164     0.51  1.70   0.67  0.26    0.27            0.05             0.77

 177       0.01      2,4,6-TRICHLOROPHENOL   88062
 196     0.58  1.97   0.76  0.30    0.91            0.05             0.88
 198     0.58  1.99   0.77  0.30    0.32            0.06             0.89

 178       0.01      DI-TERT-BUTYL-4-METHYLPHENOL   128370
 205     1.85  6.13   2.37  0.92    0.96            0.17             2.73
 220     0.49  1.61   0.62  0.24    0.25            0.05             0.72
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             Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56         Std #57         Std #58
Mass     109   236    136    -       82    128       98    116       84    112


 179        0.01    PENTACHLOROPHENOL  87865
 264     0.29  0.22  0.05           0.34  0.54     0.19  0.31     0.72  0.52
 266     0.47  0.36  0.09           0.55  0.91     0.32  0.54     1.17  0.84

 180        0.01    FLUORENE 86737
 165     2.74  2.13  0.49           3.01  4.85     1.95  3.27     6.12  4.50
 166     3.07  2.38  0.57           3.44  5.55     2.23  3.74     6.99  5.14

 181        0.01    2,3,5-TRIMETHYLNAPHTHALENE    2245387
 155     1.86  1.44  0.34           2.08  3.36     1.36  2.27     4.24  3.12
 170     2.56  1.99  0.47           2.86  4.62     1.86  3.11     5.83  4.29

 182        0.01    ANTHRACENE  120127
 178     3.21  2.47  0.60           3.71  5.74     2.04  3.38     7.43  5.30

 183        0.01    PYRENE  129000
 202     4.88  3.75  0.95           5.66  8.73     3.27  5.18    11.54  8.23

 184        0.01    9,10-DIMETHYLANTHRACENE    781431
 191     1.33  1.03  0.25           1.45  2.35     0.94  1.57     2.96  2.18
 206     2.85  2.22  0.53           3.13  5.04     2.01  3.37     6.36  4.68

 185        0.01    CHRYSENE  218019
 228     2.21  1.73  0.41           2.42  3.92     1.59  2.66     4.91  3.61

 186        0.01    PERYLENE  198550
 252     1.60  1.23  0.30           1.84  2.86     1.02  1.68     3.67  2.62

 187        0.01    DICYANOBUTANE  111693
  41     0.66  0.51  0.12           0.72  1.17     0.47  0.79     1.47  1.08
  54     0.29  0.23  0.05           0.32  0.52     2.10  0.35     0.66  0.48

 188        0.01    BUTYLCARBAMATE 14994775
  41     0.48  0.36  0.08           0.54  0.86     0.28  0.47     1.35  1.00
  59     0.24  0.26  0.05           0.29  0.47     0.15  0.25     0.72  0.54

 189        0.01    BIS(2-CHLOROETHYL)ETHANE     112265
  63     1.71  1.31  0.31           1.97  3.13     1.03  1.71     4.91  3.63
  93     0.84  0.65  0.15           0.97  1.54     0.51  0.84     2.42  1.78

 190        0.01    TRIBUTYLPHOSPHATE  126738
  99     4.03  3.10  0.75           4.65  7.20     2.56  4.24     9.28  6.62
 155     0.88  0.68  0.16           1.01  1.57     0.56  0.92     2.02  1.44

 191        0.01    DIHYDROBENZOFURAN(2,3)  496162
  91     0.68  0.52  0.13           0.79  1.25     0.43  0.72     1.58  1.13
 120     0.97  0.75  0.18           1.12  1.67     0.66  0.78     2.16  1.54

 192        0.01    NITROBENZENE   98953
  77     0.86  0.67  0.16           0.94  1.51     0.61  1.02     1.91  1.40
 123     0.54  0.42  0.10           0.59  0.95     0.38  0.64     1.20  0.88
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              Internal/External Standard File for Cmpd Class # 4

     Cmpd#    Recovery   Compound Name
               Std #59      Std #60      Std #61       Std #62        Std #63
     Mass     110   125    82   110     264    -      188     -       99     -


      179       0.01      PENTACHLOROPHENOL  87865
     264     0.20  0.68   0.28  0.11    0.11          0.02           0.31
     266     0.36  1.11   0.45  0.07    0.18          0.04           0.50

      180       0.01      FLUORENE 86737
     165     2.00  6.62   2.57  0.99    1.04          0.19           2.95
     166     2.28  7.57   2.93  1.14    1.19          0.21           3.38

      181       0.01      2,3,5-TRIMETHYLNAPHTHALENE   2245387
     155     1.38  4.59   1.78  0.69    0.72          0.13           2.05
     170     1.90  6.31   2.44  0.95    0.99          0.18           2.81

      182       0.01      ANTHRACENE  120127
     178     2.24  7.59   3.08  1.19    1.13          0.25           3.35

      183       0.01      PYRENE  129000
     202     3.59 11.47   4.95  1.90    1.80          0.40           5.36

      184       0.01      9,10-DIMETHYLANTHRACENE   781431
     191     0.96  3.19   1.24  0.48    0.50          0.09           1.42
     206     2.06  6.86   2.67  1.03    1.08          0.19           3.06

      185       0.01      CHRYSENE  218019
     228     1.61  5.34   2.07  0.80    0.81          0.15           2.39

      186       0.01      PERYLENE  198550
     252     1.11  3.72   1.53  0.59    0.47          0.12           1.65

      187       0.01      DICYANOBUTANE  111693
      41     0.48  1.59   0.62  0.24    0.25          0.05           0.71
      54     0.22  0.71   0.28  0.11    0.11          0.02           0.32

      188       0.01      BUTYLCARBAMATE 14994775
      41     0.35  1.16   0.50  0.09    0.15          0.04           0.52
      59     0.19  0.63   0.27  0.11    0.08          0.02           0.28

      189       0.01      BIS(2-CHLOROETHYL)ETHANE    112265
      63     1.27  4.23   1.83  0.71    0.56          0.13           1.91
      93     0.61  2.08   0.90  0.35    0.27          0.06           0.94

      190       0.01      TRIBUTYLPHOSPHATE  126738
      99     2.81  9.43   3.87  1.49    1.41          0.31           4.19
     155     0.61  2.05   0.84  0.32    0.31          0.07           0.91

      191       0.01      DIHYDROBENZOFURAN(2,3)  496162
      91     0.27  1.59   0.65  0.25    0.24          0.05           0.71
     120     0.68  2.27   0.90  0.35    0.33          0.07           0.98

      192       0.01      NITROBENZENE    98953
      77     0.61  2.07   0.80  0.31    0.33          0.06           0.94
     123     0.38  1.30   0.50  0.20    0.21          0.04           0.59
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             Internal/External Standard File for Cmpd Class # 4

  Cmpd#    Recovery    Compound Name
            Std # 2       Std #54        Std #56        Std #57        Std #58
  Mass     109   236     136    -        82   128       98   116       84   112


   193       0.01      BEANZOTHIAZOLE  95169
   135     1.56  1.21   0.29           1.71  2.76     1.11  1.86     3.47  2.55

   194       0.01      PHENYLCARBAMATE   102090
    94     1.25  0.96   0.23           1.44  2.23     0.79  1.31     2.88  2.06
   137     0.02  0.01   0.00           0.02  0.03     0.01  0.02     0.04  0.03

   195       0.01      2,4-DINITROTOLUENE 121142
    89     0.35  0.28   0.06           0.40  0.65     0.26  0.44     0.81  0.60
   165     0.71  0.53   0.13           0.75  1.21     0.46  0.76     1.53  1.13

   196       0.01      BENZYLSULFIDE   538749
    91     3.55  2.68   0.63           4.00  6.38     2.10  3.49     9.99  7.42
   123     0.90  0.68   0.16           1.02  1.62     0.53  0.89     2.54  1.88

   197       0.01      DIPHENYLSULFONE 127639
   125     3.82  3.44   0.81           5.16  8.21     2.71  4.51    12.95  8.65
   218     0.92  0.73   0.17           1.10  1.75     0.58  0.96     2.74  2.03

   198       0.01      TRIPHENYLPHOSPHATE    115866
   325     2.59  2.01   0.13           0.79  1.28     0.52  0.87     1.61  1.18
   326     0.09  0.07   0.17           1.03  1.67     0.68  1.14     2.09  1.54

   199       0.01      DIPHENYLMERCURY 587859
    77     0.72  0.56   0.48           2.85  4.59     1.96  3.28     6.08  4.47
   356     0.95  0.74   0.02           0.09  0.15     0.06  0.11     0.20  0.15

   200       0.01      TETRAPHENYLTIN
   197     1.40  1.13   0.27           1.70  2.71     0.89  1.47     4.21  3.13
   351     1.30  1.05   0.25           1.58  2.51     0.82  1.37     3.91  2.91

   201       0.82      BENZYLCHLORIDE 100447
    91     1.55  1.18   0.28           1.77  2.82     0.93  1.54     4.42  3.28
   126     0.42  0.32   0.08           0.48  0.76     0.25  0.42     1.20  0.89

   202       0.01      4-CHLOROBENZONITRILE 623030
   102     0.55  0.42   0.10           0.63  0.99     0.33  0.55     1.57  1.16
   137     2.10  1.57   0.36           2.38  3.79     1.25  2.08     5.95  4.40

   203       0.01      3-CHLOROBENZALDEHYDE  587042
   111     0.06  0.05   0.01           0.08  0.12     0.04  0.07     0.20  0.14
   139     0.12  0.10   0.02           0.15  0.24     0.08  0.13     0.38  0.28

   204       0.01      O-CHLOROANISOLE  766518
   127     0.60  0.46   0.11           0.69  1.09     0.36  0.60     1.71  1.27
   142     1.32  1.00   0.24           0.50  2.40     0.79  1.31     3.76  2.78

   205       0.01      CHLOROBENZAMIDE 619567
   139     0.70  0.55   0.13           0.77  1.25     0.50  0.84     1.57  1.16
   155     0.38  0.30   0.07           0.42  0.68     0.27  0.46     0.85  0.63
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              Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std #59      Std #60      Std #61        Std #62        Std #63
Mass     110   125     82   110    264    -       188    -        99    -


 193       0.01     BEANZOTHIAZOLE  95169
 135    1.14  3.76   1.46  0.57   0.59            0.11            1.68

 194       0.01     PHENYLCARBAMATE   102090
  94    0.87  2.92   1.20  0.46   0.44            0.10            1.30
 137    0.01  0.04   0.01  0.01   0.00            0.00            0.02

 195       0.01     2,4-DINITROTOLUENE 121142
  89    0.27  0.88   0.34  0.13   0.14            0.03            0.39
 165    0.50  1.66   0.64  0.25   0.26            0.05            0.74

 196       0.01     BENZYLSULFIDE   538749
  91    2.47  8.62   3.72  1.44   1.11            0.27            3.90
 123    0.63  2.19   0.94  0.37   0.28            0.07            0.99

 197       0.01     DIPHENYLSULFONE 127639
 125    3.00 11.09   4.77  1.85   1.22            0.35            5.05
 218    0.67  2.36   1.02  0.29   0.30            0.07            1.07

 198       0.01     TRIPHENYLPHOSPHATE   115866
 325    1.98  6.58   2.55  0.95   1.03            0.18            0.78
 326    0.06  0.22   0.08  0.03   0.03            0.01            1.02

 199       0.01     DIPHENYLMERCURY 587859
  77    0.53  1.75   0.68  0.26   0.26            0.05            2.94
 356    0.69  2.28   0.88  0.34   0.35            0.06            0.10

 200       0.01     TETRAPHENYLTIN
 197    1.10  3.66   1.57  0.61   0.44            0.11            1.56
 351    1.03  3.40   1.46  0.57   0.41            0.11            1.54

 201       0.82     BENZYLCHLORIDE 100447
  91    1.10  3.81   1.64  0.64   0.50            0.12            1.71
 126    0.30  1.03   0.45  0.17   0.12            0.03            0.47

 202       0.01     4-CHLOROBENZONITRILE 623030
 102    0.39  1.35   0.58  0.23   0.18            0.04            0.61
 137    1.49  5.12   2.21  0.85   0.67            0.16            2.32

 203       0.01     3-CHLOROBENZALDEHYDE  587042
 111    0.05  0.17   0.07  0.03   0.02            0.00            0.08
 139    0.10  0.32   0.14  0.05   0.04            0.01            0.15

 204       0.01     O-CHLOROANISOLE  766518
 127    0.43  1.48   0.64  0.25   0.17            0.05            0.67
 142    0.94  3.24   1.40  0.54   0.36            0.10            1.46

 205       0.01     CHLOROBENZAMIDE 619567
 139    0.51  1.70   0.66  0.26   0.27            0.05            0.76
 155    0.26  0.92   0.36  0.14   0.15            0.03            0.41
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           Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass     109   236    136     -      82   128      98   116      84   112


  206       0.01     3,4-DICHLOROBENZALDEHYDE  6287383
 173    0.48  0.39    0.09          0.58  0.93    0.31  0.57    1.46  1.07
 174    0.32  0.26    0.06          0.39  0.62    0.21  0.34    0.98  0.72

  207       0.01     1,2,4-TRICHLOROBENZENE 120821
 145    0.34  0.26    0.06          0.40  0.63    0.22  0.36    0.80  0.57
 180    1.30  1.00    0.24          1.50  2.40    0.83  1.37    3.03  2.16

  208       0.01     2-BROMO-1-CHLOROBENZENE  694804
 190    0.78  0.61    0.14          0.85  1.38    0.55  0.92    1.74  1.28
 192    1.04  0.81    0.19          1.14  1.84    0.74  1.24    2.33  1.71

  209       0.68     1,2-DICHLORONAPHTHALENE  2050693
 161    0.44  0.34    0.08          0.50  0.78    0.28  0.46    1.01  0.72
 196    2.17  1.67    0.40          2.51  3.88    1.38  2.29    5.03  3.58

  210       0.53     1,2,4,5-TETRACHLOROBENZENE    95943
 214    1.18  0.90    0.22          1.29  2.09    0.84  1.40    2.63  1.94
 216    1.54  1.18    0.28          1.69  2.72    1.09  1.83    3.43  2.52

  211       0.43     P-DIBROMOBENZENE    106376
 234    0.68  0.52    0.12          0.77  1.23    0.41  0.67    1.93  1.43
 236    1.29  1.00    0.23          1.48  2.36    0.78  1.30    3.77  2.93

  212       0.01     4-BROMODIPHENYLETHER  6452499
 248    1.08  0.81    0.20          1.19  1.92    0.77  1.29    2.42  1.78
 250    1.13  0.88    0.21          1.26  2.04    0.82  1.37    2.57  1.89

  213       0.95     HEXACHLOROBENZENE    118741
 284    0.74  0.56    0.13          0.84  1.34    0.44  0.73    2.10  1.55
 286    0.60  0.46    0.11          0.68  1.08    0.36  0.59    1.70  1.26
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            Internal/External Standard File for Cmpd Class # 4

Cmpd#    Recovery   Compound Name
          Std #59     Std #60       Std #61       Std #62        Std #63
Mass     110   125    82   110      264    -      188    -        99    -


  206       0.01     3,4-DICHLOROBENZALDEHYDE  6287383
  173    0.37  1.25   0.54  0.21    0.17          0.04           0.57
  174    0.25  0.84   0.36  0.14    0.11          0.03           0.38

  207       0.01     1,2,4-TRICHLOROBENZENE 120821
  145    0.24  0.80   0.33  0.13    0.12          0.03           0.36
  180    0.89  3.05   1.25  0.48    0.46          0.10           1.36

  208       0.01     2-BROMO-1-CHLOROBENZENE  694804
  190    0.57  1.88   0.73  0.28    0.30          0.05           0.84
  192    0.76  2.52   0.98  0.38    0.40          0.07           1.12

  209       0.68     1,2-DICHLORONAPHTHALENE  2050693
  161    0.31  1.02   0.42  0.16    0.15          0.03           0.46
  196    1.52  5.08   2.08  0.80    0.76          0.17           2.27

  210       0.53     1,2,4,5-TETRACHLOROBENZENE   95943
  214    0.86  2.85   1.11  0.43    0.45          0.08           1.27
  216    1.12  3.72   1.44  0.56    0.58          0.11           1.66

  211       0.43     P-DIBROMOBENZENE   106376
  234    0.49  1.66   0.72  0.28    0.19          0.05           0.75
  236    0.93  3.18   1.38  0.53    0.45          0.10           1.45

  212       0.01     4-BROMODIPHENYLETHER  6452499
  248    0.79  2.61   1.01  0.39    0.41          0.07           1.17
  250    0.84  2.78   1.08  0.42    0.44          0.08           1.24

  213       0.95     HEXACHLOROBENZENE     118741
  284    0.53  1.83   0.78  0.30    0.24          0.06           0.82
  286    0.43  1.46   0.63  0.24    0.19          0.05           0.66
```

Table B-5. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NOS. 2 & 3)

Class No. 5

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	0.66	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	NA	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	NA	1.03(a)	.60(0)	-	.18(6)	1.07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	0.40	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	0.55	.97(4)	.57(10)	.95(10)	.16(3)	-	1.60(1)	2.35(17)	1.70(16)
	128	0.55	.61(2)	.35(9)	.59(9)	.10(1)	.63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	84	0.62	.42(15)	.25(24)	.42(24)	.071 [illegible](18)	.44(16)	.70(15)	-	.73(2)
	112	0.62	.58(15)	.35(22)	.58(23)	.098(18)	.61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	0.42	1.09(4)	.65(13)	1.07(14)	.18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	0.42	2.85(5)	1.67(13)	2.78(14)	.48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	ND	1.52(2)	.90(7)	1.50(8)	.25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	ND	.46(2)	.27(8)	.45(7)	~~.26~~(3) .076	.48(3)	.76(4)	1.11(18)	.81(17)
d_{12}-perylene	264	0.78	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	0.77	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	NA	1.10(4)	.65(7)	1.08(8)	.18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	NA	1.43(4)	.84(6)	1.39(7)	.24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(continued)

			Standard							
			d_5-Propiophenone		d_5-Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-Iodotoluene	
Compound	Ion	Recovery	*m*/*z* 82	*m*/*z* 110	*m*/*z* 110	*m*/*z* 125	*m*/*z* 264	*m*/*z* 188	*m*/*z* 109	*m*/*z* 236
d_5-phenol	99	0.66	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-*o*-xylene	98	NA	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	NA	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	0.40	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	0.55	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	0.55	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	0.62	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	0.62	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	0.42	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	0.42	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	ND	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	ND	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	0.78	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	0.77	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

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            Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54        Std #56        Std #57        Std #58
Mass     109   236     136     -      82   128       98   116       84   112


 100       0.49      ALPHA-PICOLINE     109068
  66     0.26  0.20   0.05           0.30  0.46     0.16  0.27     0.59  0.42
  93     0.66  0.51   0.12           0.76  1.18     0.40  0.66     1.52  1.09

 101       0.63      ANILINE  62533
  66     0.23  0.19   0.04           0.28  0.41     0.15  0.24     0.53  0.38
  93     0.76  0.54   0.13           0.81  1.25     0.45  0.74     1.62  1.15

 102       0.44      INDOLE    120729
  90     0.72  0.54   0.13           0.82  1.30     0.43  0.71     2.04  1.51
 117     1.92  1.45   0.34           2.17  3.46     1.14  1.89     5.43  4.02

 103       0.60      2,3,6-TRIMETHYLPYRIDINE    1462846
 120     0.66  0.51   0.12           0.76  1.18     0.42  0.69     1.53  1.09
 121     0.90  0.69   0.17           1.03  1.61     0.55  0.91     2.08  1.49

 104       0.86      2,6-DIMETHYLANILINE    1300738
 106     0.36  0.27   0.06           0.41  0.65     0.21  0.36     1.02  0.75
 121     0.57  0.44   0.10           0.66  1.04     0.34  0.57     1.64  1.21

 105       0.80      M-CHLOROANILINE    108429
 127     1.09  0.84   0.20           1.26  1.94     0.69  1.15     2.52  1.79
 129     0.34  0.26   0.06           0.29  0.60     0.22  0.36     0.78  0.56

 106       0.53      QUINOLINE    91225
 129     1.82  1.41   0.34           1.99  3.22     1.30  2.17     4.06  2.98

 107       0.55      2,4-DIMETHYLQUINOLINE  1198374
 156     0.41  0.32   0.08           0.47  0.75     0.26  0.43     0.95  0.68
 157     2.01  1.54   0.37           2.31  3.59     1.27  2.11     4.64  3.31

 108       0.73      CARBAZOLE       87648
 167     3.73  2.88   0.69           4.30  6.66     2.37  3.92     9.36  6.67

 109       0.55      2-AMINOBIPHENYL   90415
 168     6.79  5.11   1.20           7.65 12.18     4.61  6.67    19.13 14.17
 169    12.72  9.45   2.22          14.15 22.54     7.42 12.30    35.40 26.19

 110       0.87      DIPHENYLAMINE  122394
 168     1.48  1.14   0.27           1.71  2.65     0.94  1.56     3.43  2.45
 169     2.79  2.15   0.52           3.22  4.99     1.77  2.93     6.45  4.60

 111       0.40      TRIBUTYLAMINE  102829
 100     0.42  0.33   0.08           0.49  0.75     0.27  0.44     0.97  0.69
 142     1.53  1.18   0.28           1.77  2.74     0.97  1.61     3.52  2.51

 112       0.68      CAFFEINE  58082
 109     0.10  0.08   0.02           0.12  0.17     0.06  0.10     0.23  0.16
 194     0.19  0.15   0.04           0.22  0.34     0.12  0.20     0.44  0.32

 113       0.43      DIBENZYLAMINE     103491
  91     1.62  1.26   0.30           1.78  2.87     1.16  1.94     3.63  2.67
 197     0.13  0.11   0.03           0.15  0.24     0.10  0.16     0.30  0.22
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              Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std #59       Std #60       Std #61        Std #62        Std #63
Mass     110   125      82   110      264     -      188     -       99     -


 100       0.49      ALPHA-PICOLINE    109068
  66    0.18  0.60    0.25  0.09    0.09           0.02           0.27
  93    0.46  1.54    0.63  0.24    0.23           0.05           0.69

 101       0.63      ANILINE  62533
  66    0.17  0.56    0.22  0.09    0.08           0.02           0.24
  93    0.49  1.64    0.67  0.26    0.24           0.05           0.73

 102       0.44      INDOLE   120729
  90    0.51  1.75    0.76  0.29    0.23           0.05           0.79
 117    1.40  4.68    2.02  0.78    0.61           0.15           2.12

 103       0.60      2,3,6-TRIMETHYLPYRIDINE   1462846
 120    0.46  1.54    0.63  0.24    0.23           0.05           0.67
 121    0.62  2.10    0.86  0.33    0.32           0.07           0.94

 104       0.86      2,6-DIMETHYLANILINE   1300738
 106    0.26  0.88    0.38  0.15    0.11           0.03           0.40
 121    0.42  1.41    0.61  0.24    0.18           0.04           0.64

 105       0.80      M-CHLOROANILINE   108429
 127    0.76  2.55    1.05  0.40    0.38           0.98           1.14
 129    0.24  0.79    0.33  0.13    0.12           0.03           0.35

 106       0.53      QUINOLINE    91225
 129    1.33  4.40    1.70  0.66    0.69           0.12           1.96

 107       0.55      2,4-DIMETHYLQUINOLINE  1198374
 156    0.29  0.96    0.40  0.15    0.15           0.03           0.43
 157    1.46  4.69    1.93  0.74    0.71           0.15           2.09

 108       0.73      CARBAZOLE       87648
 167    2.60  8.72    3.57  1.37    1.28           0.31           4.22

 109       0.55      2-AMINOBIPHENYL   90415
 168    4.75 16.46    7.10  2.75    2.13           0.51           7.45
 169    8.82 30.44   13.14  5.08    3.96           0.95          13.80

 110       0.87      DIPHENYLAMINE  122394
 168    1.03  3.47    1.42  0.55    0.52           0.11           1.55
 169    1.94  6.46    2.68  1.03    0.98           0.22           2.91

 111       0.40      TRIBUTYLAMINE  102829
 100    0.29  0.99    0.41  0.16    0.15           0.03           0.44
 142    0.99  3.34    1.47  0.57    0.53           0.12           1.59

 112       0.68      CAFFEINE  58082
 109    0.07  0.23    0.09  0.04    0.04           0.01           0.10
 194    0.13  0.45    0.18  0.07    0.07           0.02           0.21

 113       0.43      DIBENZYLAMINE     103491
  91    1.18  3.91    1.52  0.59    0.62           0.11           1.74
 197    0.10  0.32    0.13  0.05    0.05           0.01           0.14
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              Internal/External Standard File for Cmpd Class # 5

   Cmpd#    Recovery   Compound Name
             Std # 2     Std #54        Std #56        Std #57        Std #58
   Mass     109   236   136    -       82    128      98    116       84    112


    114       0.74     N,N-DIMETHYLDODECYLAMINE    112185
     58    4.72  3.88   0.87           5.47  8.83    3.58  5.99   11.09  8.16
     59    0.17  0.13   0.03           0.20  0.30    0.13  0.21    0.40  0.29

    115       0.78     ATRAZINE    1912249
    200    2.75  2.20   0.52           3.28  5.23    1.72  2.86    8.17  6.09
    215    1.67  1.34   0.31           2.00  3.18    1.05  1.74    4.97  3.71

    116       0.55     HEPTANONE(2) 110430
     43    1.21  0.94   0.22           1.33  2.14    0.85  1.14    2.32  2.00
     58    0.75  0.58   0.14           0.83  1.33    0.53  0.88    1.69  1.25

    117       0.70     BUTOXYETHANOL    111762
     41    0.21  0.17   0.04           0.25  0.40    0.13  0.22    0.49  0.35
     57    0.55  0.42   0.10           0.63  1.03    0.35  0.58    1.27  0.91

    118       0.55     2-OCTANONE   111137
     43    1.30  1.01   0.24           1.43  2.31    0.91  1.53    2.92  2.15
     58    1.02  0.79   0.19           1.11  1.80    0.71  1.19    2.27  1.67

    119       0.31     BUTYLPROPIONATE   590012
     57    1.48  1.14   0.27           1.71  2.73    0.90  1.49    4.27  3.15
     75    0.44  0.34   0.08           0.51  0.82    0.27  0.45    1.28  0.95

    120       0.71     ISOPHOBRONE   78591
     82    1.77  1.36   0.33           2.04  3.17    1.13  1.86    4.11  2.93
    138    0.39  0.30   0.07           0.45  0.72    0.25  0.41    0.90  0.64

    121       0.63     FENCHONE   1195759
     69    0.66  0.51   0.12           0.72  1.17    0.47  0.78    1.47  1.08
     81    1.44  1.12   0.27           1.58  2.55    1.02  1.71    3.22  2.36

    122       1.11     ALPHA-TERPINEOL   98555
     59    0.56  0.43   0.10           0.65  1.00    0.36  0.59    1.31  0.93
    136    0.32  0.25   0.06           0.37  0.58    0.21  0.34    0.75  0.53

    123       0.71     N-DECANOL    112301
     41    0.40  0.31   0.07           0.46  0.74    0.25  0.42    0.92  0.66
     43    0.44  0.34   0.08           0.51  0.79    0.28  0.46    1.02  0.73

    124       0.49     DIMETHYLADIPATE 627930
     59    0.56  0.45   0.10           0.64  1.03    0.41  0.69    1.29  0.95
    114    0.44  0.35   0.08           0.49  0.79    0.32  0.54    1.00  0.74

    125       0.91     METHYLSTEARATE 112618
     74    3.42  2.65   0.63           3.89  6.28    2.54  4.25    7.90  5.81
     87    2.22  1.72   0.41           2.52  4.07    1.65  2.76    5.13  3.77

    126       0.32     PHENYLACETATE    122792
     94    1.84  1.43   0.34           2.01  3.25    1.30  2.18    4.10  3.01
    136    0.25  0.20   0.05           0.28  0.45    0.18  0.30    0.57  0.42
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              Internal/External Standard File for Cmpd Class # 5

Cmpd#     Recovery    Compound Name
           Std #59      Std #60       Std #61         Std #62         Std #63
Mass      110   125     82    110     264     -       188     -       99     -


  114        0.74     N,N-DIMETHYLDODECYLAMINE       112185
   58     3.62 12.02   4.66  1.81     1.87            0.34            5.37
   59     0.13  0.43   0.17  0.06     0.07            0.01            0.19

  115        0.78     ATRAZINE    1912249
  200     2.13  7.07   3.05  1.18     0.90            0.22            3.26
  215     1.21  4.30   1.85  0.72     0.55            0.13            1.95

  116        0.55     HEPTANONE(2) 110430
   43     0.88  2.91   1.13  0.44     0.47            0.08            1.30
   58     0.55  1.82   0.71  0.27     0.29            0.05            0.81

  117        0.70     BUTOXYETHANOL    111762
   41     0.15  0.49   0.20  0.09     0.07            0.02            0.22
   57     0.38  1.28   0.52  0.20     0.19            0.04            0.57

  118        0.55     2-OCTANONE   111137
   43     0.95  3.14   1.22  0.47     0.51            0.09            1.40
   58     0.74  2.45   0.95  0.37     0.39            0.07            1.09

  119        0.31     BUTYLPROPIONATE  590012
   57     1.11  3.69   1.59  0.61     0.48            0.12            1.66
   75     0.33  1.11   0.48  0.19     0.15            0.04            0.50

  120        0.71     ISOPHOBRONE  78591
   82     1.23  4.14   1.70  0.65     0.62            0.14            1.80
  138     0.27  0.91   0.37  0.14     0.14            0.03            0.41

  121        0.63     FENCHONE  1195759
   69     0.48  1.58   0.62  0.24     0.25            0.05            0.71
   81     1.05  3.45   1.35  0.52     0.55            0.10            1.55

  122        1.11     ALPHA-TERPINEOL  98555
   59     0.39  1.31   0.54  0.21     0.20            0.04            0.58
  136     0.23  0.76   0.31  0.12     0.11            0.03            0.34

  123        0.71     N-DECANOL   112301
   41     0.28  0.93   0.38  0.15     0.14            0.03            0.41
   43     0.31  1.63   0.42  0.16     0.15            0.03            0.46

  124        0.49     DIMETHYLADIPATE 627930
   59     0.42  1.40   0.54  0.21     0.22            0.04            0.62
  114     0.33  1.08   0.42  0.16     0.17            0.03            0.48

  125        0.91     METHYLSTEARATE 112618
   74     2.58  8.56   3.32  1.29     1.33            0.24            3.83
   87     1.67  5.55   2.15  0.83     0.87            0.16            2.48

  126        0.32     PHENYLACETATE   122792
   94     1.31  4.43   1.72  0.67     0.70            0.13            1.98
  136     0.18  0.62   0.24  0.09     0.10            0.02            0.28
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             Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56        Std #57        Std #58
Mass     109   236   136    -        82   128       98   116       84   112


 127       0.55     BENZYLACETATE   140114
  91    0.52  0.40   0.09          0.57  0.92     0.37  0.62     1.15  0.85
 108    1.09  0.85   0.20          1.19  1.92     0.77  1.29     2.43  1.79

 128       0.60     DIMETHYLPHTHALATE  131113
  77    0.81  0.63   0.15          0.94  1.45     0.52  0.85     1.88  1.34
 163    5.29  4.07   0.98          6.10  9.46     3.36  5.56    12.22  8.71

 129       0.70     ETHYLTOLUENESULFONATE(P)  80400
  91    1.74  1.32   0.31          1.97  3.14     1.03  1.72     4.92  3.65
 155    1.18  0.94   0.22          1.40  2.23     0.73  1.21     3.46  2.35

 130       0.89     DIETHYLPHTHALATE  84662
 149    3.19  2.43   0.57          3.65  5.79     1.90  3.17     9.08  6.71
 177    0.80  0.61   0.14          0.93  1.47     0.48  0.80     2.29  1.69

 131       1.38     DIBUTYLPHTHALATE   84742
  57    0.29  0.23   0.05          0.34  0.52     0.19  0.31     0.68  0.48
 149    7.17  5.52   1.33          8.27 12.80     4.55  7.54    16.55 11.80

 132       0.74     BUTYLBENZYLPHTHALATE
  91    2.09  1.62   0.38          2.28  3.69     1.48  2.48     4.64  3.41
 149    3.37  2.62   0.62          3.69  5.95     2.40  4.01     7.49  5.51

 133       1.04     DIETHYLHEXYLPHTHALATE    117817
 149    5.22  4.07   0.96          5.71  9.23     3.74  6.26    11.59  8.53
 167    1.98  1.54   0.37          2.17  3.51     1.42  2.37     4.40  3.24

 134       0.43     BENZALDEHYDE      100527
  77    0.36  0.28   0.07          0.42  0.64     0.23  0.38     0.84  0.60
 105    0.40  0.31   0.07          0.46  0.70     0.25  0.42     0.92  0.66

 135       1.05     TOLUALDEHYDE      529204
  91    0.54  0.44   0.10          0.65  1.04     0.34  0.57     1.65  1.21
 119    0.63  0.51   0.12          0.77  1.23     0.41  0.68     1.95  1.43

 136       0.01     ACETOPHENONE    98862
  77    0.38  0.64   0.15          0.96  1.53     0.53  0.87     1.93  1.37
 105    1.22  0.94   0.23          1.41  2.25     0.78  1.29     2.85  2.03

 137       0.67     SALICYLALDEHYDE  90028
 121    0.56  0.44   0.10          0.61  0.99     0.40  0.67     1.24  0.91
 122    0.60  0.47   0.11          0.60  1.07     0.43  0.72     1.34  0.99

 138       0.72     ANISALDEHYDE  123115
 135    1.37  1.08   0.25          1.53  2.47     0.91  1.66     3.11  2.29
 136    0.96  0.76   0.18          1.07  1.73     0.70  1.16     2.18  1.60

 139       0.61     PHENOL     108952
  94    1.07  0.84   0.20          1.18  1.90     0.76  1.27     2.41  1.77
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               Internal/External Standard File for Cmpd Class # 5

Cmpd#   Recovery    Compound Name
         Std #59      Std #60      Std #61        Std #62        Std #63
Mass    110   125    82    110    264     -      188     -       99     -


 127      0.55     BENZYLACETATE    140114
  91   0.38  1.25   0.48  0.19    0.20          0.04          0.56
 108   0.79  2.63   1.02  0.40    0.41          0.07          1.17

 128      0.60     DIMETHYLPHTHALATE  131113
  77   0.57  1.83   0.75  0.29    0.28          0.06          0.85
 163   3.68 11.87   4.88  1.88    1.85          0.41          5.51

 129      0.70     ETHYLTOLUENESULFONATE(P)  80400
  91   1.28  4.25   1.83  0.71    0.55          0.13          1.92
 155   0.91  3.01   1.30  0.50    0.38          0.09          1.36

 130      0.89     DIETHYLPHTHALATE  84662
 149   2.35  7.82   3.34  1.30    1.02          0.24          3.54
 177   0.59  1.97   0.85  0.33    0.26          0.06          0.89

 131      1.38     DIBUTYLPHTHALATE   84742
  57   0.20  0.68   0.28  0.11    0.10          0.02          0.31
 149   4.99 16.75   6.88  2.64    2.52          0.55          7.47

 132      0.74     BUTYLBENZYLPHTHALATE
  91   1.51  5.02   1.95  0.76    0.78          0.14          2.24
 149   2.44  8.10   3.15  1.22    1.26          0.23          3.62

 133      1.04     DIETHYLHEXYLPHTHALATE    117817
 149   4.03 12.58   4.88  1.89    1.90          0.35          5.61
 167   1.53  4.78   1.85  0.72    0.72          0.13          2.13

 134      0.43     BENZALDEHYDE      100527
  77   0.25  0.84   0.35  0.13    0.13          0.03          0.38
 105   0.28  0.93   0.38  0.15    0.14          0.03          0.42

 135      1.05     TOLUALDEHYDE      529204
  91   0.42  1.41   0.61  0.24    0.15          0.05          0.64
 119   0.50  1.66   0.72  0.28    0.22          0.05          0.75

 136      0.01     ACETOPHENONE    98862
  77   0.57  1.95   0.80  0.31    0.29          0.06          0.87
 105   0.85  2.88   1.18  0.45    0.43          0.09          1.28

 137      0.67     SALICYLALDEHYDE  90028
 121   0.41  1.35   0.52  0.20    0.21          0.04          0.60
 122   0.44  1.46   0.56  0.22    0.23          0.04          0.65

 138      0.72     ANISALDEHYDE  123115
 135   1.01  3.36   1.30  0.51    0.53          0.09          1.50
 136   0.71  2.36   0.91  0.35    0.37          0.07          1.05

 139      0.61     PHENOL     108952
  94   0.75  2.60   1.01  0.39    0.41          0.07          1.15
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              Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56       Std #57       Std #58
Mass     109   236   136    -        82   128      98   116      84   112


 140       0.62     CRESOL(P)   106445
 107     1.21  0.93  0.23           1.40  2.25    0.80  1.29    2.91  2.08
 108     1.07  0.82  0.20           1.24  1.99    0.69  1.14    2.58  1.84

 141       0.58     2,3-DIMETHYLPHENOL  526750
 107     0.87  0.67  0.16           1.00  1.61    0.57  0.95    2.08  1.48
 122     0.91  0.70  0.17           1.05  1.64    0.58  0.96    2.12  1.51

 142       0.57     ISOPROPYLPHENOL  88699
 121     1.79  1.36  0.32           2.04  3.25    1.07  1.78    5.10  3.77
 136     0.07  0.56  0.12           0.75  1.19    0.39  0.65    1.87  1.38

 143       0.49     O-NITROPHENOL   88755
  65     0.03  0.02  0.00           0.03  0.05    0.02  0.03    0.06  0.05
 139     0.13  0.10  0.02           0.14  0.23    0.09  0.15    0.29  0.21

 144       1.18     4-CHLORO-3-METHYLPHENOL     59507
 107     0.93  0.71  0.17           1.06  1.68    0.55  0.92    2.64  2.95
 142     1.02  0.77  0.18           1.16  1.84    0.61  1.01    2.89  2.14

 145       0.89     1-NAPHTHOL  90153
 115     0.35  0.26  0.06           0.38  0.61    0.20  0.34    0.96  0.72
 144     0.61  0.45  0.11           0.67  1.07    0.35  0.29    1.68  1.25

 146       0.77     P-TERT-BUTYLPHENOL   98544
 107     0.56  0.43  0.10           0.65  1.03    0.34  0.56    1.60  1.18
 135     1.96  1.49  0.35           2.22  3.54    1.17  1.94    5.56  4.11

 147       0.61     2-NITROCRESOL     119335
  77     0.26  0.20  0.05           0.30  0.46    0.07  0.27    0.60  0.43
 153     0.74  0.57  0.14           0.83  1.33    0.46  0.78    1.72  1.23

 148       0.81     2,4-DICHLOROPHENOL  120832
 162     1.13  0.88  0.21           1.24  2.00    0.80  1.34    2.52  1.86
 164     0.72  0.53  0.13           0.78  1.27    0.51  0.85    1.60  1.18

 149       0.30     2,4,6-TRICHLOROPHENOL     88062
 196     0.81  0.63  0.15           0.89  1.44    0.58  0.97    1.88  1.34
 198     0.83  0.64  0.15           0.91  1.46    0.59  0.98    1.90  1.36

 150       0.69     DI-TERT-BUTYL-4-METHYLPHENOL     128370
 205     2.53  1.97  0.47           2.78  4.49    1.81  3.03    5.66  4.16
 220     0.67  0.52  0.12           0.73  1.18    0.48  0.80    1.49  1.09

 151       0.48     2-METHYLNAPHTHALENE    91576
 141     2.03  1.58  0.38           2.23  3.60    1.44  2.42    4.53  3.34
 142     2.51  1.96  0.46           2.76  4.45    1.79  2.99    5.62  4.13

 152       0.50     ACENAPHTHENE     83329
 153     1.26  0.98  0.23           1.38  2.22    0.89  1.49    2.81  2.06
 154     3.40  2.64  0.63           3.73  6.02    2.41  4.04    7.59  5.58
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```
              Internal/External Standard File for Cmpd Class # 5

  Cmpd#     Recovery     Compound Name
             Std #59        Std #60        Std #61           Std #62           Std #63
  Mass      110    125     82    110      264     -          188    -          99     -


   140        0.62       CRESOL(P)    106445
  107     0.88   2.85    1.17   0.45    0.44              0.10              1.31
  108     0.78   2.52    1.03   0.40    0.39              0.09              1.16

   141        0.58       2,3-DIMETHYLPHENOL   526750
  107     0.63   2.11    0.84   0.32    0.32              0.07              0.94
  122     0.64   2.14    0.85   0.33    0.32              0.07              0.95

   142        0.57       ISOPROPYLPHENOL   88699
  121     1.28   4.39    1.90   0.73    0.58              0.14              1.99
  136     0.47   1.61    0.69   0.27    0.21              0.05              0.73

   143        0.49       O-NITROPHENOL    88755
   65     0.02   0.07    0.03   0.01    0.01              0.00              0.03
  139     0.09   0.31    0.12   0.05    0.05              0.01              0.14

   144        1.18       4-CHLORO-3-METHYLPHENOL      59507
  107     0.66   2.27    0.98   0.38    0.30              0.07              1.03
  142     0.72   2.49    1.07   0.42    0.32              0.08              1.13

   145        0.89       1-NAPHTHOL   90153
  115     0.25   0.83    0.36   0.14    0.11              0.03              0.38
  144     0.44   1.45    0.62   0.24    0.18              0.05              0.66

   146        0.77       P-TERT-BUTYLPHENOL    98544
  107     0.40   1.38    0.66   0.23    0.18              0.04              0.62
  135     1.44   4.79    2.04   0.80    0.63              0.15              2.16

   147        0.61       2-NITROCRESOL     119335
   77     0.18   0.61    0.25   0.10    0.09              0.02              0.27
  153     0.52   1.74    0.71   0.27    0.26              0.06              0.78

   148        0.81       2,4-DICHLOROPHENOL   120832
  162     0.80   2.73    1.05   0.41    0.43              0.08              1.22
  164     0.51   1.70    0.67   0.26    0.27              0.05              0.77

   149        0.30       2,4,6-TRICHLOROPHENOL      88062
  196     0.58   1.97    0.76   0.30    0.91              0.05              0.86
  198     0.58   1.99    0.77   0.30    0.32              0.06              0.89

   150        0.69       DI-TERT-BUTYL-4-METHYLPHENOL      128370
  205     1.85   6.13    2.37   0.92    0.96              0.17              2.73
  220     0.49   1.61    0.62   0.24    0.25              0.05              0.72

   151        0.48       2-METHYLNAPHTHALENE    91576
  141     1.48   4.91    1.90   0.74    0.77              0.14              2.19
  142     1.78   6.08    2.36   0.91    0.95              0.17              2.71

   152        0.50       ACENAPHTHENE     83329
  153     0.92   3.04    1.18   0.46    0.47              0.09              1.35
  154     2.48   8.22    3.19   1.23    1.28              0.23              3.66
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```
           Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56       Std #57       Std #58
Mass     109   236    136    -       82   128      98   116      84   112


 153       0.84     FLUORENE 86737
 165    2.74  2.13   0.49          3.01  4.85   1.95  3.27    6.12  4.50
 166    3.07  2.38   0.57          3.44  5.55   2.23  3.74    6.99  5.14

 154       0.48     2,3,5-TRIMETHYLNAPHTHALENE     2245387
 155    1.86  1.44   0.34          2.08  3.36   1.36  2.27    4.24  3.12
 170    2.56  1.99   0.47          2.86  4.62   1.86  3.11    5.83  4.29

 155       0.66     ANTHRACENE    120127
 178    3.21  2.47   0.60          3.71  5.74   2.04  3.38    7.43  5.30

 156       0.78     PYRENE      129000
 202    4.88  3.75   0.95          5.66  8.73   3.27  5.18   11.54  8.23

 157       0.63     9,10-DIMETHYLANTHRACENE  781431
 191    1.33  1.03   0.25          1.45  2.35   0.94  1.57    2.96  2.18
 206    2.85  2.22   0.53          3.13  5.04   2.01  3.37    6.36  4.68

 158       0.95     CHRYSENE   218019
 228    2.21  1.73   0.41          2.42  3.92   1.59  2.66    4.91  3.61

 159       1.18     PERYLENE   198550
 252    1.60  1.23   0.30          1.84  2.86   1.02  1.68    3.67  2.62

 160       1.04     DICYANOBUTANE  111693
  41    0.66  0.51   0.12          0.72  1.17   0.47  0.79    1.47  1.08
  54    0.29  0.23   0.05          0.32  0.52   2.10  0.35    0.66  0.48

 161       0.65     BIS(2-CHLOROETHYL)ETHANE     112265
  63    1.71  1.31   0.31          1.97  3.13   1.03  1.71    4.91  3.63
  93    0.84  0.65   0.15          0.97  1.54   0.51  0.84    2.42  1.78

 162       0.75     TRIBUTYLPHOSPHATE     126738
  99    4.03  3.10   0.75          4.65  7.20   2.56  4.24    9.28  6.62
 155    0.88  0.68   0.16          1.01  1.57   0.56  0.92    2.02  1.44

 163       0.48     DIHYDROBENZOFURAN(2,3)     496162
  91    0.68  0.52   0.13          0.79  1.25   0.43  0.72    1.58  1.13
 120    0.97  0.75   0.18          1.12  1.67   0.66  0.78    2.16  1.54

 164       0.58     NITROBENZENE     98953
  77    0.86  0.67   0.16          0.94  1.51   0.61  1.02    1.91  1.40
 123    0.54  0.42   0.10          0.59  0.95   0.38  0.64    1.20  0.88

 165       0.58     BENZOTHIAZOLE    95169
 135    1.56  1.21   0.29          1.71  2.76   1.11  1.86    3.47  2.55

 166       0.48     PHENYLCARBAMATE       102090
  94    1.25  0.96   0.23          1.44  2.23   0.79  1.31    2.88  2.06
 137    0.02  0.01   0.00          0.02  0.03   0.01  0.02    0.04  0.03
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              Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std #59       Std #60       Std #61       Std #62       Std #63
Mass     110   125     82   110     264     -      188     -      99     -


 153       0.84      FLUORENE 86737
165     2.00  6.62   2.57  0.99   1.04          0.19          2.95
166     2.28  7.57   2.93  1.14   1.19          0.21          3.38

 154       0.48      2,3,5-TRIMETHYLNAPHTHALENE    2245387
155     1.38  4.59   1.78  0.69   0.72          0.13          2.05
170     1.90  6.31   2.44  0.95   0.99          0.18          2.81

 155       0.66      ANTHRACENE    120127
178     2.24  7.59   3.08  1.19   1.13          0.25          3.35

 156       0.78      PYRENE       129000
202     3.59 11.47   4.95  1.90   1.80          0.40          5.36

 157       0.63      9,10-DIMETHYLANTHRACENE  781431
191     0.96  3.19   1.24  0.48   0.50          0.09          1.42
206     2.06  6.86   2.67  1.03   1.08          0.19          3.06

 158       0.95      CHRYSENE   218019
228     1.61  5.34   2.07  0.80   0.81          0.15          2.39

 159       1.18      PERYLENE   198550
252     1.11  3.72   1.53  0.59   0.47          0.12          1.65

 160       1.04      DICYANOBUTANE  111693
 41     0.48  1.59   0.62  0.24   0.25          0.05          0.71
 54     0.22  0.71   0.28  0.11   0.11          0.02          0.32

 161       0.65      BIS(2-CHLOROETHYL)ETHANE     112265
 63     1.27  4.23   1.83  0.71   0.56          0.13          1.91
 93     0.61  2.08   0.90  0.35   0.27          0.06          0.94

 162       0.75      TRIBUTYLPHOSPHATE      126738
 99     2.81  9.43   3.87  1.49   1.41          0.31          4.19
155     0.61  2.05   0.84  0.32   0.31          0.07          0.91

 163       0.48      DIHYDROBENZOFURAN(2,3)     496162
 91     0.27  1.59   0.65  0.25   0.24          0.05          0.71
120     0.68  2.27   0.90  0.35   0.33          0.07          0.98

 164       0.58      NITROBENZENE     98953
 77     0.61  2.07   0.80  0.31   0.33          0.06          0.94
123     0.38  1.30   0.50  0.20   0.21          0.04          0.59

 165       0.58      BENZOTHIAZOLE    95169
135     1.14  3.76   1.46  0.57   0.59          0.11          1.68

 166       0.48      PHENYLCARBAMATE       102090
 94     0.87  2.92   1.20  0.46   0.44          0.10          1.30
137     0.01  0.04   0.01  0.01   0.00          0.00          0.02
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```
          Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2    Std #54        Std #56        Std #57         Std #58
Mass     109   236   136     -      82    128      98    116       84    112


 167       1.05     2,4-DINITROTOLUENE      121142
  89    0.35  0.28   0.06           0.40  0.65    0.26  0.44     0.81  0.60
 165    0.71  0.53   0.13           0.75  1.21    0.46  0.76     1.53  1.13

 168       0.71     BENZYLSULFIDE     583749
  91    3.55  2.68   0.63           4.00  6.38    2.10  3.49     9.99  7.42
 123    0.90  0.68   0.16           1.02  1.62    0.53  0.89     2.54  1.88

 169       0.67     DIPHENYLSULFONE         127639
 125    3.82  3.44   0.81           5.16  8.21    2.71  4.51    12.95  8.65
 218    0.92  0.73   0.17           1.10  1.75    0.58  0.96     2.74  2.03

 170       0.71     TRIPHENYLPHOSPHATE     115866
 325    2.59  2.01   0.13           0.79  1.28    0.52  0.87     1.61  1.18
 326    0.09  0.07   0.17           1.03  1.67    0.68  1.14     2.09  1.54

 171       0.81     DIPHENYLMERCURY   587859
  77    0.72  0.56   0.48           2.85  4.59    1.96  3.28     6.08  4.47
 356    0.95  0.74   0.02           0.09  0.15    0.06  0.11     0.20  0.15

 172       0.72     TETRAPHENYLTIN
 197    1.40  1.13   0.27           1.70  2.71    0.89  1.47     4.21  3.13
 351    1.30  1.05   0.25           1.58  2.51    0.82  1.37     3.91  2.91

 173       0.01     PYRIDINE    110861
  52    0.29  0.22   0.05           0.33  0.51    0.19  0.32     0.67  0.48
  79    0.44  0.34   0.08           0.51  0.78    0.30  0.50     1.10  0.78

 174       0.01     TOLUIDINE     106490
 106    0.89  0.69   0.16           0.97  1.57    0.64  1.07     1.97  1.45
 107    0.71  0.56   0.13           0.78  1.27    0.51  0.86     1.58  1.16

 175       0.01     LUTIDINE 108485
 106    0.13  0.10   0.02           0.15  0.25    0.08  0.13     0.39  0.28
 107    0.22  0.16   0.04           0.24  0.39    0.13  0.21     0.61  0.45

 176       0.01     P-NITROANILINE  100016
  65    0.44  0.35   0.08           0.52  0.83    0.27  0.46     1.30  0.97
 138    0.56  0.45   0.11           0.67  1.07    0.35  0.58     1.68  0.22

 177       0.01     NICOTINE     54155
  84    1.17  0.90   0.22           1.35  2.09    0.74  1.23     2.70  1.92
 133    0.28  0.21   0.05           0.32  0.49    0.17  0.29     0.63  0.45

 178       0.01     DICYCLOHEXYLAMINE    101837
  56    0.33  0.37   0.06           0.39  0.63    0.21  0.35     1.10  0.78
 138    0.96  0.76   0.18           1.12  1.80    0.61  1.02     3.15  2.25

 179       0.01     N-DECANE    124185
  43    1.47  1.11   0.26           1.67  2.66    0.88  1.46     4.18  3.09
  57    1.42  1.08   0.25           1.64  2.61    0.85  1.41     4.05  3.00
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```
               Internal/External Standard File for Cmpd Class # 5

Cmpd#     Recovery    Compound Name
           Std #59       Std #60        Std #61        Std #62        Std #63
Mass      110    125     82    110     264     -      188     -       99     -


  167       1.05      2,4-DINITROTOLUENE      121142
   89     0.27  0.88   0.34  0.13    0.14           0.03           0.39
  165     0.50  1.66   0.64  0.25    0.26           0.05           0.74

  168       0.71      BENZYLSULFIDE    583749
   91     2.47  8.62   3.72  1.44    1.11           0.27           3.90
  123     0.63  2.19   0.94  0.37    0.28           0.07           0.99

  169       0.67      DIPHENYLSULFONE         127639
  125     3.00 11.09   4.77  1.85    1.22           0.35           5.05
  218     0.67  2.36   1.02  0.29    0.30           0.07           1.07

  170       0.71      TRIPHENYLPHOSPHATE     115866
  325     1.98  6.58   2.55  0.95    1.03           0.18           0.78
  326     0.06  0.22   0.08  0.03    0.03           0.01           1.02

  171       0.81      DIPHENYLMERCURY   587859
   77     0.53  1.75   0.68  0.26    0.26           0.05           2.94
  356     0.69  2.28   0.88  0.34    0.35           0.06           0.10

  172       0.72      TETRAPHENYLTIN
  197     1.10  3.66   1.57  0.61    0.44           0.11           1.56
  351     1.03  3.40   1.46  0.57    0.41           0.11           1.54

  173       0.01      PYRIDINE     110861
   52     0.20  0.68   0.28  0.11    0.10           0.02           0.30
   79     0.33  1.11   0.42  0.16    0.17           0.04           0.50

  174       0.01      TOLUIDINE     106490
  106     0.65  2.15   0.83  0.32    0.32           0.06           0.96
  107     0.52  1.73   0.67  0.26    0.26           0.05           0.77

  175       0.01      LUTIDINE 108485
  106     0.10  0.33   0.14  0.05    0.04           0.01           0.15
  107     0.16  0.52   0.23  0.09    0.06           0.02           0.24

  176       0.01      P-NITROANILINE  100016
   65     0.34  1.13   0.49  0.19    0.14           0.04           0.51
  138     0.43  1.84   0.62  0.24    0.19           0.05           0.65

  177       0.01      NICOTINE      54155
   84     0.82  2.74   1.12  0.43    0.41           0.09           1.22
  133     0.19  0.64   0.26  0.10    0.10           0.02           0.29

  178       0.01      DICYCLOHEXYLAMINE    101837
   56     0.25  0.81   0.33  0.14    0.09           0.03           0.38
  138     0.71  2.34   0.95  0.40    0.26           0.08           1.09

  179       0.01      N-DECANE    124185
   43     1.05  3.59   1.55  0.60    0.47           0.11           1.62
   57     1.01  3.48   1.50  0.58    0.46           0.11           1.58
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```
           Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56       Std #57       Std #58
Mass     109   236    136    -       82   128      98   116      84   112


  180      0.01     N-TRIDECANE   629505
   43    2.18  1.64   0.34          2.48  3.95    1.30  2.16    6.20  4.58
   57    2.75  2.09   0.50          3.14  5.01    1.66  2.77    7.93  5.86

  181      0.01     N-TETRADECANE   629594
   43    2.52  1.92   0.45          2.88  4.58    1.51  2.51    7.19  5.31
   57    3.40  2.55   0.61          3.87  6.16    2.03  3.37    9.67  7.15

  182      0.01     N-PENTADECANE  692629
   57    2.78  2.14   0.52          3.22  4.99    1.77  2.94    6.47  4.62
   71    1.73  1.33   0.32          2.01  3.11    1.10  1.83    4.03  2.87

  183      0.01     N-HEXADECANE     544763
   43    1.90  1.45   0.34          2.16  3.45    1.13  1.89    5.41  3.99
   57    2.72  2.08   0.49          3.11  4.96    1.63  2.71    7.78  5.74

  184      0.01     N-HEPTADECANE     629787
   57    3.13  2.41   0.58          3.61  5.59    1.99  3.30    7.25  5.17
   71    2.07  1.60   0.38          2.39  3.70    1.32  2.18    4.80  3.42

  185      0.01     N-OCTADECANE  593453
   57    2.99  2.51   0.59          3.75  5.98    1.88  3.14    8.96  6.63
   71    1.98  1.66   0.39          2.48  3.95    1.25  2.08    5.95  4.41

  186      0.01     N-NONADECANE  629952
   71    2.12  1.61   0.38          2.42  3.85    1.27  2.11    6.04  4.47
   85    1.42  1.08   0.25          1.61  2.57    0.85  1.41    4.03  2.98

  187      0.01     N-EICOSANE    1112958
   57    4.43  3.41   0.82          5.11  7.92    2.82  4.66   10.26  7.32
   71    3.03  2.33   0.56          3.50  5.43    1.93  3.19    7.03  5.01

  188      0.01     N-HENEICOSANE  629947
   57    3.93  2.96   0.70          4.43  7.05    2.32  3.86   11.05  8.20
   71    2.71  2.05   0.48          3.07  4.88    1.61  2.67    7.65  5.68

  189      0.01     N-DOCOSANE   629970
   57    3.73  2.98   0.70          4.46  7.10    2.33  3.88   11.11  8.26
   71    2.60  2.08   0.49          3.11  4.96    1.63  2.70    7.76  5.77

  190      0.01     N-TRICOSANE   638675
   57    3.99  3.19   0.75          4.77  7.60    2.49  4.14   11.85  8.83
   71    2.80  2.24   0.53          3.35  5.34    1.75  2.91    8.33  6.20

  191      0.01     METHYLBENZENESULFONATE
   77    1.24  0.94   0.22          1.41  2.25    0.74  1.23    3.54  2.61
  172    0.44  0.34   0.08          0.50  0.80    0.26  0.44    1.26  0.93

  192      0.01     METHYLTOLUENESULFONATE(P)
   91    1.60  1.21   0.29          1.81  2.89    0.95  1.58    4.53  3.35
  155    0.72  0.54   0.13          0.81  1.29    0.42  0.71    2.02  1.50
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```
               Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std #59       Std #60      Std #61         Std #62         Std #63
Mass      110   125     82   110     264    -        188    -        99    -


 180        0.01     N-TRIDECANE    629505
  43     1.56  5.33   2.30  0.89    0.70            0.17            2.41
  57     1.99  6.75   2.94  1.14    0.76            0.21            3.09

 181        0.01     N-TETRADECANE    629594
  43     1.86  6.19   2.67  1.03    0.80            0.19            2.80
  57     2.50  8.33   3.57  1.39    1.08            0.26            3.77

 182        0.01     N-PENTADECANE   692629
  57     1.94  6.52   2.68  1.03    0.99            0.22            2.92
  71     1.21  4.06   1.67  0.64    0.62            0.14            1.82

 183        0.01     N-HEXADECANE        544763
  43     1.40  4.66   2.01  0.78    0.61            0.15            2.11
  57     2.01  6.70   2.88  1.12    0.87            0.21            3.03

 184        0.01     N-HEPTADECANE        629787
  57     2.18  7.32   3.01  1.16    1.11            0.24            3.27
  71     1.44  4.85   1.99  0.77    0.73            0.16            2.17

 185        0.01     N-OCTADECANE   593453
  57     2.33  8.10   3.48  1.35    1.01            0.24            3.65
  71     1.55  5.35   2.30  0.89    0.58            0.06            2.41

 186        0.01     N-NONADECANE   629952
  71     1.51  5.27   2.24  0.87    0.68            0.16            2.35
  85     1.01  3.47   1.50  0.58    0.45            0.11            1.57

 187        0.01     N-EICOSANE     1112958
  57     3.08 10.35   4.25  1.63    1.57            0.35            4.63
  71     2.11  7.09   2.91  1.12    1.07            0.23            3.17

 188        0.01     N-HENEICOSANE  629947
  57     2.73  9.53   4.11  1.60    1.07            0.30            4.31
  71     1.89  6.60   2.85  1.10    0.74            0.21            2.99

 189        0.01     N-DOCOSANE   629970
  57     2.89  9.60   4.14  1.60    1.22            0.30            4.35
  71     2.02  6.71   2.89  1.12    0.85            0.21            3.04

 190        0.01     N-TRICOSANE    638675
  57     3.10 10.28   4.42  1.71    1.29            0.32            4.65
  71     2.18  7.22   3.11  1.20    0.90            0.22            3.27

 191        0.01     METHYLBENZENESULFONATE
  77     0.91  3.04   1.31  0.51    0.40            0.09            1.38
 172     0.32  1.08   0.47  0.18    0.14            0.03            0.49

 192        0.01     METHYLTOLUENESULFONATE(P)
  91     1.17  3.90   1.68  0.65    0.51            0.12            1.76
 155     0.52  1.74   0.75  0.29    0.23            0.05            0.79
```

```
            Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54          Std #56       Std #57       Std #58
Mass     109   236     136     -        82    128     98    116     84    112


 193        0.01     4-CHLOROCRESOL
 107    0.83  0.64    0.16             0.97  1.57   0.53  0.88    2.03  1.45
 142    0.94  0.72    0.17             1.09  1.77   0.60  0.99    2.29  1.63

 194        0.01     PENTACHLOROPHENOL      87865
 264    0.29  0.22    0.05             0.34  0.54   0.19  0.31    0.72  0.52
 266    0.47  0.36    0.09             0.55  0.91   0.32  0.54    1.17  0.84

 195        0.01     BIPHENYL  92524
 154    2.28  1.78    0.42             2.51  4.04   1.63  2.72    5.10  3.75

 196        0.01     1,8-DIMETHYLNAPHTHALENE  569415
 141    1.59  1.24    0.29             1.74  2.82   1.13  1.89    3.55  2.61
 156    2.30  1.79    0.42             2.52  4.07   1.63  2.73    5.13  3.77

 197        0.01     BUTYLCARBAMATE  14994775
  41    0.48  0.36    0.08             0.54  0.86   0.28  0.47    1.35  1.00
  59    0.24  0.26    0.05             0.29  0.47   0.15  0.25    0.72  0.54

 198        0.01     DI-T-BUTYLDISULFIDE     110065
  41    0.73  0.56    0.13             0.84  1.34   0.44  0.73    2.10  1.55
  57    3.09  2.36    0.56             3.54  5.64   1.85  3.09    8.84  6.54

 199        0.01     ALDRIN  309002
  66    1.33  1.03    0.24             1.49  2.40   0.97  1.62    3.03  2.23
 263    0.60  0.46    0.11             0.67  1.08   0.44  0.73    1.36  1.00

 200        0.01     BENZYLCHLORIDE        100447
  91    1.55  1.18    0.28             1.77  2.82   0.93  1.54    4.42  3.28
 126    0.42  0.32    0.08             0.48  0.76   0.25  0.42    1.20  0.89

 201        0.47     4-CHLOROBENZONITRILE  623030
 102    0.55  0.42    0.10             0.63  0.99   0.33  0.55    1.57  1.16
 137    2.10  1.57    0.36             2.38  3.79   1.25  2.08    5.95  4.40

 202        0.80     3-CHLOROBENZALDEHYDE  587042
 111    0.06  0.05    0.01             0.08  0.12   0.04  0.07    0.20  0.14
 139    0.12  0.10    0.02             0.15  0.24   0.08  0.13    0.38  0.28

 203        0.50     O-CHLOROANISOLE  766518
 127    0.60  0.46    0.11             0.69  1.09   0.36  0.60    1.71  1.27
 142    1.32  1.00    0.24             0.50  2.40   0.79  1.31    3.76  2.78

 204        0.01     CHLOROBENZAMIDE   619567
 139    0.70  0.55    0.13             0.77  1.25   0.50  0.84    1.57  1.16
 155    0.38  0.30    0.07             0.42  0.68   0.27  0.46    0.85  0.63

 205        0.55     3,4-DICHLOROBENZALDEHYDE  6287383
 173    0.48  0.39    0.09             0.58  0.93   0.31  0.57    1.46  1.07
 174    0.32  0.26    0.06             0.39  0.62   0.21  0.34    0.98  0.72
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          Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery    Compound Name
          Std #59      Std #60      Std #61      Std #62       Std #63
Mass     110   125     82   110    264    -     188    -        99    -


 193       0.01      4-CHLOROCRESOL
 107    0.58  1.96    0.80  0.31   0.31          0.07          0.91
 142    0.66  2.20    0.85  0.34   0.35          0.08          1.03

 194       0.01      PENTACHLOROPHENOL      87865
 264    0.20  0.68    0.28  0.11   0.11          0.02          0.31
 266    0.36  1.11    0.45  0.07   0.18          0.04          0.50

 195       0.01      BIPHENYL  92524
 154    1.67  5.52    2.14  0.83   0.87          0.16          2.46

 196       0.01      1,8-DIMETHYLNAPHTHALENE  569415
 141    1.16  3.84    1.49  0.58   0.60          0.11          1.71
 156    1.67  5.55    2.15  0.83   0.87          0.16          2.48

 197       0.01      BUTYLCARBAMATE  14994775
  41    0.35  1.16    0.50  0.09   0.15          0.04          0.52
  59    0.19  0.63    0.27  0.11   0.08          0.02          0.28

 198       0.01      DI-T-BUTYLDISULFIDE   110065
  41    0.54  1.78    0.78  0.31   0.20          0.06          0.82
  57    2.21  7.62    3.29  1.27   1.00          0.24          3.42

 199       0.01      ALDRIN  309002
  66    0.99  3.28    1.27  0.49   0.51          0.09          1.46
 263    0.44  1.47    0.57  0.22   0.23          0.04          0.66

 200       0.01      BENZYLCHLORIDE      100447
  91    1.10  3.81    1.64  0.64   0.50          0.12          1.71
 126    0.30  1.03    0.45  0.17   0.12          0.03          0.47

 201       0.47      4-CHLOROBENZONITRILE  623030
 102    0.39  1.35    0.58  0.23   0.18          0.04          0.61
 137    1.49  5.12    2.21  0.85   0.67          0.16          2.32

 202       0.80      3-CHLOROBENZALDEHYDE  587042
 111    0.05  0.17    0.07  0.03   0.02          0.00          0.08
 139    0.10  0.32    0.14  0.05   0.04          0.01          0.15

 203       0.50      O-CHLOROANISOLE  766518
 127    0.43  1.48    0.64  0.25   0.17          0.05          0.67
 142    0.94  3.24    1.40  0.54   0.36          0.10          1.46

 204       0.01      CHLOROBENZAMIDE   619567
 139    0.51  1.70    0.66  0.26   0.27          0.05          0.76
 155    0.28  0.92    0.36  0.14   0.15          0.03          0.41

 205       0.55      3,4-DICHLOROBENZALDEHYDE  6287383
 173    0.37  1.25    0.54  0.21   0.17          0.04          0.57
 174    0.25  0.84    0.36  0.14   0.11          0.03          0.38
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          Internal/External Standard File for Cmpd Class # 5

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56       Std #57       Std #58
Mass     109   236    136    -      82   128      98   116      84   112


 206       1.07     1,2,4-TRICHLOROBENZENE   120821
 145    0.34  0.26   0.06          0.40  0.63   0.22  0.36   0.80  0.57
 180    1.30  1.00   0.24          1.50  2.40   0.83  1.37   3.03  2.16

 207       0.01     2-BROMO-1-CHLOROBENZENE        694804
 190    0.78  0.61   0.14          0.85  1.38   0.55  0.92   1.74  1.28
 192    1.04  0.81   0.19          1.14  1.84   0.74  1.24   2.33  1.71

 208       0.68     1,2-DICHLORONAPHTHALENE   2050693
 161    0.44  0.34   0.08          0.50  0.78   0.28  0.46   1.01  0.72
 196    2.17  1.67   0.40          2.51  3.88   1.38  2.29   5.03  3.58

 209       0.53     1,2,4,5-TETRACHLOROBENZENE         95943
 214    1.18  0.90   0.22          1.29  2.09   0.84  1.40   2.63  1.94
 216    1.54  1.18   0.28          1.69  2.72   1.09  1.83   3.43  2.52

 210       0.43     P-DIBROMOBENZENE       106376
 234    0.68  0.52   0.12          0.77  1.23   0.41  0.67   1.93  1.43
 236    1.29  1.00   0.23          1.48  2.36   0.78  1.30   3.77  2.93

 211       0.80     4-BROMODIPHENYLETHER      6452499
 248    1.08  0.81   0.20          1.19  1.92   0.77  1.29   2.42  1.78
 250    1.13  0.88   0.21          1.26  2.04   0.82  1.37   2.57  1.89

 212       0.95     HEXACHLOROBENZENE       118741
 284    0.74  0.56   0.13          0.84  1.34   0.44  0.73   2.10  1.55
 286    0.60  0.46   0.11          0.68  1.08   0.36  0.59   1.70  1.26
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                 Internal/External Standard File for Cmpd Class # 5

Cmpd#     Recovery    Compound Name
           Std #59        Std #60        Std #61        Std #62        Std #63
Mass      110    125    82    110      264      -      188      -      99      -


  206       1.07      1,2,4-TRICHLOROBENZENE    120821
 145     0.24  0.80   0.33  0.13    0.12           0.03           0.36
 180     0.89  3.05   1.25  0.48    0.46           0.10           1.36

  207       0.01      2-BROMO-1-CHLOROBENZENE         694804
 190     0.57  1.88   0.73  0.28    0.30           0.05           0.84
 192     0.76  2.52   0.98  0.38    0.40           0.07           1.12

  208       0.68      1,2-DICHLORONAPHTHALENE    2050693
 161     0.31  1.02   0.42  0.16    0.15           0.03           0.46
 196     1.52  5.08   2.08  0.80    0.76           0.17           2.27

  209       0.53      1,2,4,5-TETRACHLOROBENZENE        95943
 214     0.86  2.85   1.11  0.43    0.45           0.08           1.27
 216     1.12  3.72   1.44  0.56    0.58           0.11           1.66

  210       0.43      P-DIBROMOBENZENE       106376
 234     0.49  1.66   0.72  0.28    0.19           0.05           0.75
 236     0.93  3.18   1.38  0.53    0.45           0.10           1.45

  211       0.80      4-BROMODIPHENYLETHER       6452499
 248     0.79  2.61   1.01  0.39    0.41           0.07           1.17
 250     0.84  2.78   1.08  0.42    0.44           0.08           1.24

  212       0.95      HEXACHLOROBENZENE       118741
 284     0.53  1.83   0.78  0.30    0.24           0.06           0.82
 286     0.43  1.46   0.63  0.24    0.19           0.05           0.66
```

Table B-6. RMRs AND RECOVERIES FOR WABN COMPOUNDS
(BLLE, pH 8.0/FRACTION NO. 3)

Class No. 6

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Standard							
		d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
		m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	1.03(a)	.60(0)	-	.18(6)	1.07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	.97(4)	.57(10)	.95(10)	.16(3)	-	1.60(1)	2.35(17)	1.70(16)
	128	.61(2)	.35(9)	.59(9)	.10(1)	.63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	84	.42(15)	.25(24)	.42(24)	.071 ~~.71~~(18)	.44(16)	.70(15)	-	.73(2)
	112	.58(15)	.35(22)	.58(23)	.098(18)	.61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	1.09(4)	.65(13)	1.07(14)	.18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	2.85(5)	1.67(13)	2.78(14)	.48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	1.52(2)	.90(7)	1.50(8)	.25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	.46(2)	.27(8)	.45(7)	~~.76~~(3) .076	.48(3)	.76(4)	1.11(18)	.81(17)
d_{12}-perylene	264	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	1.10(4)	.65(7)	1.08(8)	.18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	1.43(4)	.84(6)	1.39(7)	.24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(continued)

Compound	Ion	Standard							
		d_5-Propiophenone		d_5-Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-Iodotoluene	
		m/z 82	*m/z* 110	*m/z* 110	*m/z* 125	*m/z* 264	*m/z* 188	*m/z* 109	*m/z* 236
d_5-phenol	99	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-*o*-xylene	98	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

[a] (CV).

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            Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery     Compound Name
          Std # 2       Std #54       Std #56       Std #57       Std #58
Mass     109   236      136    -     82   128      98   116      84   112


  100       0.01      PYRIDINE 110861
   52    0.29  0.22    0.05          0.33  0.51    0.19  0.32    0.67  0.48
   79    0.44  0.34    0.08          0.51  0.78    0.30  0.50    1.10  0.78

  101       0.01      ALPHA-PICOLINE 109068
   66    0.26  0.20    0.05          0.30  0.46    0.16  0.27    0.59  0.42
   93    0.66  0.51    0.12          0.76  1.18    0.40  0.66    1.52  1.09

  102       0.01      ANILINE   62533
   66    0.23  0.19    0.04          0.28  0.41    0.15  0.24    0.53  0.38
   93    0.76  0.54    0.13          0.81  1.25    0.45  0.74    1.62  1.15

  103       0.01      LUTIDINE  108485
  106    0.13  0.10    0.02          0.15  0.25    0.08  0.13    0.39  0.28
  107    0.22  0.16    0.04          0.24  0.39    0.13  0.21    0.61  0.45

  104       0.01      TOLUIDINE(P)  106490
  106    0.89  0.69    0.16          0.97  1.57    0.64  1.07    1.97  1.45
  107    0.71  0.56    0.13          0.78  1.27    0.51  0.86    1.58  1.16

  105       0.01      INDOLE  120729
   90    0.72  0.54    0.13          0.82  1.30    0.43  0.71    2.04  1.51
  117    1.92  1.45    0.34          2.17  3.46    1.14  1.89    5.43  4.02

  106       0.01      2,3,6-TRIMETHYLPYRIDINE     1462846
  120    0.66  0.51    0.12          0.76  1.18    0.42  0.69    1.53  1.09
  121    0.90  0.69    0.17          1.03  1.61    0.55  0.91    2.08  1.49

  107       0.01      2,6-DIMETHYLANILINE 1300738
  106    0.36  0.27    0.06          0.41  0.65    0.21  0.36    1.02  0.75
  121    0.57  0.44    0.10          0.66  1.04    0.34  0.57    1.64  1.21

  108       0.01      M-CHLOROANILINE 108429
  127    1.09  0.84    0.20          1.26  1.94    0.69  1.15    2.52  1.79
  129    0.34  0.26    0.06          0.29  0.60    0.22  0.36    0.78  0.56

  109       0.01      QUINOLINE 91225
  129    1.82  1.41    0.34          1.99  3.22    1.30  2.17    4.06  2.98

  110       0.01      P-NITROANILINE     100016
   65    0.44  0.35    0.08          0.52  0.83    0.27  0.46    1.30  0.97
  138    0.56  0.45    0.11          0.67  1.07    0.35  0.58    1.68  0.22

  111       0.01      2,4-DIMETHYLQUINOLINE 1198374
  156    0.41  0.32    0.08          0.47  0.75    0.26  0.43    0.95  0.68
  157    2.01  1.54    0.37          2.31  3.59    1.27  2.11    4.64  3.31

  113       0.01      NICOTINE   54115
   84    1.17  0.90    0.22          1.35  2.09    0.74  1.23    2.70  1.92
  133    0.28  0.21    0.05          0.32  0.49    0.17  0.29    0.63  0.45
```

```
                Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std #59      Std #60       Std #61        Std #62        Std #63
Mass      110   125     82   110     264     -      188     -       99     -


 100        0.01      PYRIDINE 110861
  52     0.20  0.68    0.28  0.11    0.10           0.02           0.30
  79     0.33  1.11    0.42  0.16    0.17           0.04           0.50

 101        0.01      ALPHA-PICOLINE 109068
  66     0.18  0.60    0.25  0.09    0.09           0.02           0.27
  93     0.46  1.54    0.63  0.24    0.23           0.05           0.69

 102        0.01      ANILINE   62533
  66     0.17  0.56    0.22  0.09    0.08           0.02           0.24
  93     0.49  1.64    0.67  0.26    0.24           0.05           0.73

 103        0.01      LUTIDINE  108485
 106     0.10  0.33    0.14  0.05    0.04           0.01           0.15
 107     0.16  0.52    0.23  0.09    0.06           0.02           0.24

 104        0.01      TOLUIDINE(P)  106490
 106     0.65  2.15    0.83  0.32    0.32           0.06           0.96
 107     0.52  1.73    0.67  0.26    0.26           0.05           0.77

 105        0.01      INDOLE  120729
  90     0.51  1.75    0.76  0.29    0.23           0.05           0.79
 117     1.40  4.68    2.02  0.78    0.61           0.15           2.12

 106        0.01      2,3,6-TRIMETHYLPYRIDINE     1462846
 120     0.46  1.54    0.63  0.24    0.23           0.05           0.67
 121     0.62  2.10    0.86  0.33    0.32           0.07           0.94

 107        0.01      2,6-DIMETHYLANILINE 1300738
 106     0.26  0.88    0.38  0.15    0.11           0.03           0.40
 121     0.42  1.41    0.61  0.24    0.18           0.04           0.64

 108        0.01      M-CHLOROANILINE 108429
 127     0.76  2.55    1.05  0.40    0.38           0.98           1.14
 129     0.24  0.79    0.33  0.13    0.12           0.03           0.35

 109        0.01      QUINOLINE 91225
 129     1.33  4.40    1.70  0.66    0.69           0.12           1.96

 110        0.01      P-NITROANILINE    100016
  65     0.34  1.13    0.49  0.19    0.14           0.04           0.51
 138     0.43  1.84    0.62  0.24    0.19           0.05           0.65

 111        0.01      2,4-DIMETHYLQUINOLINE 1198374
 156     0.29  0.96    0.40  0.15    0.15           0.03           0.43
 157     1.46  4.69    1.93  0.74    0.71           0.15           2.09

 113        0.01      NICOTINE   54115
  84     0.82  2.74    1.12  0.43    0.41           0.09           1.22
 133     0.19  0.64    0.26  0.10    0.10           0.02           0.29
```

```
              Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56       Std #57       Std #58
Mass      109   236   136    -       82   128      98   116       84   112


 114        0.01     CARBAZOLE  86748
 167     3.73  2.88   0.69          4.30  6.66    2.37  3.92    9.36  6.67

 115        0.01     2-AMINOBIPHENYL   90445
 168     6.79  5.11   1.20          7.65 12.18    4.61  6.67   19.13 14.17
 169    12.72  9.45   2.22         14.15 22.54    7.42 12.30   35.40 26.19

 116        0.01     DIPHENYLAMINE     122394
 168     1.48  1.14   0.27          1.71  2.65    0.94  1.56    3.43  2.45
 169     2.79  2.15   0.52          3.22  4.99    1.77  2.93    6.45  4.60

 117        0.01     DICYCLOHEXYLAMINE      101837
  56     0.33  0.37   0.06          0.39  0.63    0.21  0.35    1.10  0.78
 138     0.96  0.76   0.18          1.12  1.80    0.61  1.02    3.15  2.25

 118        0.01     TRIBUTYLAMINE       102829
 100     0.42  0.33   0.08          0.49  0.75    0.27  0.44    0.97  0.69
 142     1.53  1.18   0.28          1.77  2.74    0.97  1.61    3.52  2.51

 119        0.01     CAFFEINE  58082
 109     0.10  0.08   0.02          0.12  0.17    0.06  0.10    0.23  0.16
 194     0.19  0.15   0.04          0.22  0.34    0.12  0.20    0.44  0.32

 120        0.01     DIBENZYLAMINE   103491
  91     1.62  1.26   0.30          1.78  2.87    1.16  1.94    3.63  2.67
 197     0.13  0.11   0.03          0.15  0.24    0.10  0.16    0.30  0.22

 121        0.01     N,N-DIMETHYLDODECYLAMINE 112185
  58     4.72  3.88   0.87          5.47  8.83    3.58  5.99   11.09  8.16
  59     0.17  0.13   0.03          0.20  0.30    0.13  0.21    0.40  0.29

 122        0.01     ATRAZINE 1912249
 200     2.75  2.20   0.52          3.28  5.23    1.72  2.86    8.17  6.09
 215     1.67  1.34   0.31          2.00  3.18    1.05  1.74    4.97  3.71

 123        0.01     HEPTANONE(2)      110430
  43     1.21  0.94   0.22          1.33  2.14    0.85  1.14    2.32  2.00
  58     0.75  0.58   0.14          0.83  1.33    0.53  0.88    1.69  1.25

 124        0.01     BUTOXYETHANOL    111762
  41     0.21  0.17   0.04          0.25  0.40    0.13  0.22    0.49  0.35
  57     0.55  0.42   0.10          0.63  1.03    0.35  0.58    1.27  0.91

 125        0.01     2-OCTANONE      111137
  43     1.30  1.01   0.24          1.43  2.31    0.91  1.53    2.92  2.15
  58     1.02  0.79   0.19          1.11  1.80    0.71  1.19    2.27  1.67

 126        0.01     BUTYLPROPIONATE     590012
  57     1.48  1.14   0.27          1.71  2.73    0.90  1.49    4.27  3.15
  75     0.44  0.34   0.08          0.51  0.82    0.27  0.45    1.28  0.95
```

```
              Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std #59      Std #60      Std #61      Std #62      Std #63
Mass      110  125      82  110     264   -      188   -       99   -


 114        0.01      CARBAZOLE  86748
 167     2.60  8.72    3.57  1.37    1.28          0.31          4.22

 115        0.01      2-AMINOBIPHENYL   90445
 168     4.75 16.46    7.10  2.75    2.13          0.51          7.45
 169     8.82 30.44   13.14  5.08    3.96          0.95         13.80

 116        0.01      DIPHENYLAMINE    122394
 168     1.03  3.47    1.42  0.55    0.52          0.11          1.55
 169     1.94  6.46    2.68  1.03    0.98          0.22          2.91

 117        0.01      DICYCLOHEXYLAMINE      101837
  56     0.25  0.81    0.33  0.14    0.09          0.03          0.38
 138     0.71  2.34    0.95  0.40    0.26          0.08          1.09

 118        0.01      TRIBUTYLAMINE      102829
 100     0.29  0.99    0.41  0.16    0.15          0.03          0.44
 142     0.99  3.34    1.47  0.57    0.53          0.12          1.59

 119        0.01      CAFFEINE  58082
 109     0.07  0.23    0.09  0.04    0.04          0.01          0.10
 194     0.13  0.45    0.18  0.07    0.07          0.02          0.21

 120        0.01      DIBENZYLAMINE   103491
  91     1.18  3.91    1.52  0.59    0.62          0.11          1.74
 197     0.10  0.32    0.13  0.05    0.05          0.01          0.14

 121        0.01      N,N-DIMETHYLDODECYLAMINE 112185
  58     3.62 12.02    4.66  1.81    1.87          0.34          5.37
  59     0.13  0.43    0.17  0.06    0.07          0.01          0.19

 122        0.01      ATRAZINE 1912249
 200     2.13  7.07    3.05  1.18    0.90          0.22          3.26
 215     1.21  4.30    1.85  0.72    0.55          0.13          1.95

 123        0.01      HEPTANONE(2)      110430
  43     0.88  2.91    1.13  0.44    0.47          0.08          1.30
  58     0.55  1.82    0.71  0.27    0.29          0.05          0.81

 124        0.01      BUTOXYETHANOL   111762
  41     0.15  0.49    0.20  0.09    0.07          0.02          0.22
  57     0.38  1.28    0.52  0.20    0.19          0.04          0.57

 125        0.01      2-OCTANONE      111137
  43     0.95  3.14    1.22  0.47    0.51          0.09          1.40
  58     0.74  2.45    0.95  0.37    0.39          0.07          1.09

 126        0.01      BUTYLPROPIONATE     590012
  57     1.11  3.69    1.59  0.61    0.48          0.12          1.66
  75     0.33  1.11    0.48  0.19    0.15          0.04          0.50
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```
           Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54      Std #56      Std #57      Std #58
Mass     109   236    136    -     82   128     98   116     84   112


 127       0.01     ISOPHORONE 78591
  82    1.77  1.36   0.33        2.04  3.17   1.13  1.86   4.11  2.93
 138    0.39  0.30   0.07        0.45  0.72   0.25  0.41   0.90  0.64

 128       0.01     FENCHONE  1195759
  69    0.66  0.51   0.12        0.72  1.17   0.47  0.78   1.47  1.08
  81    1.44  1.12   0.27        1.58  2.55   1.02  1.71   3.22  2.36

 129       0.01     ALPHA-TERPINEOL      98555
  59    0.56  0.43   0.10        0.65  1.00   0.36  0.59   1.31  0.93
 136    0.32  0.25   0.06        0.37  0.58   0.21  0.34   0.75  0.53

 130       0.01     N-DECANOL      112301
  41    0.40  0.31   0.07        0.46  0.74   0.25  0.42   0.92  0.66
  43    0.44  0.34   0.08        0.51  0.79   0.28  0.46   1.02  0.73

 131       0.01     DIMETHYLADIPATE      627930
  59    0.56  0.45   0.10        0.64  1.03   0.41  0.69   1.29  0.95
 114    0.44  0.35   0.08        0.49  0.79   0.32  0.54   1.00  0.74

 132       0.01     METHYLSTEARATE   112618
  74    3.42  2.65   0.63        3.89  6.28   2.54  4.25   7.90  5.81
  87    2.22  1.72   0.41        2.52  4.07   1.65  2.76   5.13  3.77

 133       0.01     N-DECANE    124185
  43    1.47  1.11   0.26        1.67  2.66   0.88  1.46   4.18  3.09
  57    1.42  1.08   0.25        1.64  2.61   0.85  1.41   4.05  3.00

 134       0.01     N-TRIDECANE      629505
  43    2.18  1.64   0.34        2.48  3.95   1.30  2.16   6.20  4.58
  57    2.75  2.09   0.50        3.14  5.01   1.66  2.77   7.93  5.86

 135       0.01     N-TETRADECANE      629594
  43    2.52  1.92   0.45        2.88  4.58   1.51  2.51   7.19  5.31
  57    3.40  2.55   0.61        3.87  6.16   2.03  3.37   9.67  7.15

 136       0.01     N-PENTADECANE   692629
  57    2.78  2.14   0.52        3.22  4.99   1.77  2.94   6.47  4.62
  71    1.73  1.33   0.32        2.01  3.11   1.10  1.83   4.03  2.87

 137       0.01     N-HEXADECANE   544763
  43    1.90  1.45   0.34        2.16  3.45   1.13  1.89   5.41  3.99
  57    2.72  2.08   0.49        3.11  4.96   1.63  2.71   7.78  5.74

 138       0.01     N-HEPTADECANE   629787
  57    3.13  2.41   0.58        3.61  5.59   1.99  3.30   7.25  5.17
  71    2.07  1.60   0.38        2.39  3.70   1.32  2.18   4.80  3.42

 139       0.01     N-OCTADECANE      593453
  57    2.99  2.51   0.59        3.75  5.98   1.88  3.14   8.96  6.63
  71    1.98  1.66   0.39        2.48  3.95   1.25  2.08   5.95  4.41
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```
          Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std #59     Std #60     Std #61      Std #62      Std #63
Mass     110   125    82   110    264    -     188    -      99    -


 127      0.01      ISOPHORONE 78591
  82   1.23  4.14   1.70  0.65   0.62          0.14         1.80
 138   0.27  0.91   0.37  0.14   0.14          0.03         0.41

 128      0.01      FENCHONE  1195759
  69   0.48  1.58   0.62  0.24   0.25          0.05         0.71
  81   1.05  3.45   1.35  0.52   0.55          0.10         1.55

 129      0.01      ALPHA-TERPINEOL     98555
  59   0.39  1.31   0.54  0.21   0.20          0.04         0.58
 136   0.23  0.76   0.31  0.12   0.11          0.03         0.34

 130      0.01      N-DECANOL       112301
  41   0.28  0.93   0.38  0.15   0.14          0.03         0.41
  43   0.31  1.63   0.42  0.16   0.15          0.03         0.46

 131      0.01      DIMETHYLADIPATE      627930
  59   0.42  1.40   0.54  0.21   0.22          0.04         0.62
 114   0.33  1.08   0.42  0.16   0.17          0.03         0.48

 132      0.01      METHYLSTEARATE   112618
  74   2.58  8.56   3.32  1.29   1.33          0.24         3.83
  87   1.67  5.55   2.15  0.83   0.87          0.16         2.48

 133      0.01      N-DECANE     124185
  43   1.05  3.59   1.55  0.60   0.47          0.11         1.62
  57   1.01  3.48   1.50  0.58   0.46          0.11         1.58

 134      0.01      N-TRIDECANE        629505
  43   1.56  5.33   2.30  0.89   0.70          0.17         2.41
  57   1.99  6.75   2.94  1.14   0.76          0.21         3.09

 135      0.01      N-TETRADECANE        629594
  43   1.86  6.19   2.67  1.03   0.80          0.19         2.80
  57   2.50  8.33   3.57  1.39   1.08          0.26         3.77

 136      0.01      N-PENTADECANE    692629
  57   1.94  6.52   2.68  1.03   0.99          0.22         2.92
  71   1.21  4.06   1.67  0.64   0.62          0.14         1.82

 137      0.01      N-HEXADECANE    544763
  43   1.40  4.66   2.01  0.78   0.61          0.15         2.11
  57   2.01  6.70   2.88  1.12   0.87          0.21         3.03

 138      0.01      N-HEPTADECANE   629787
  57   2.18  7.32   3.01  1.16   1.11          0.24         3.27
  71   1.44  4.85   1.99  0.77   0.73          0.16         2.17

 139      0.01      N-OCTADECANE       593453
  57   2.33  8.10   3.48  1.35   1.01          0.24         3.65
  71   1.55  5.35   2.30  0.89   0.58          0.06         2.41
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        Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56       Std #57       Std #58
Mass      109   236   136    -      82    128     98    116     84    112


  140       0.01     N-NONADECANE       629925
  71     2.12  1.61   0.38          2.42  3.85    1.27  2.11    6.04  4.47
  85     1.42  1.08   0.25          1.61  2.57    0.85  1.41    4.03  2.98

  141       0.01     N-EICOSANE 1112958
  57     4.43  3.41   0.82          5.11  7.92    2.82  4.66   10.26  7.32
  71     3.03  2.33   0.56          3.50  5.43    1.93  3.19    7.03  5.01

  142       0.01     N-HENEICOSANE  629947
  57     3.93  2.96   0.70          4.43  7.05    2.32  3.86   11.05  8.20
  71     2.71  2.05   0.48          3.07  4.88    1.61  2.67    7.65  5.68

  143       0.01     N-DOCOSANE 629970
  57     3.73  2.98   0.70          4.46  7.10    2.33  3.88   11.11  8.26
  71     2.60  2.08   0.49          3.11  4.96    1.63  2.70    7.76  5.77

  144       0.01     N-TRICOSANE  638675
  57     3.99  3.19   0.75          4.77  7.60    2.49  4.14   11.85  8.83
  71     2.80  2.24   0.53          3.35  5.34    1.75  2.91    8.33  6.20

  145       0.01     PHENYLACETATE   122792
  94     1.84  1.43   0.34          2.01  3.25    1.30  2.18    4.10  3.01
 136     0.25  0.20   0.05          0.28  0.45    0.18  0.30    0.57  0.42

  146       0.01     BENZYLACETATE    140114
  91     0.52  0.40   0.09          0.57  0.92    0.37  0.62    1.15  0.85
 108     1.09  0.85   0.20          1.19  1.92    0.77  1.29    2.43  1.79

  147       0.01     METHYLBENZENESULFONATE
  77     1.24  0.94   0.22          1.41  2.25    0.74  1.23    3.54  2.61
 172     0.44  0.34   0.08          0.50  0.80    0.26  0.44    1.26  0.93

  148       0.01     METHYLTOLUENESULFONATE(P)
  91     1.60  1.21   0.29          1.81  2.89    0.95  1.58    4.53  3.35
 155     0.72  0.54   0.13          0.81  1.29    0.42  0.71    2.02  1.50

  149       0.01     DIMETHYLPHTHALATE      131113
  77     0.81  0.63   0.15          0.94  1.45    0.52  0.85    1.88  1.34
 163     5.29  4.07   0.98          6.10  9.46    3.36  5.56   12.22  8.71

  150       0.01     ETHYLTOLUENESULFONATE(P)  80400
  91     1.74  1.32   0.31          1.97  3.14    1.03  1.72    4.92  3.65
 155     1.18  0.94   0.22          1.40  2.23    0.73  1.21    3.46  2.35

  151       0.01     DIETHYLPHTHALATE 84662
 149     3.19  2.43   0.57          3.65  5.79    1.90  3.17    9.08  6.71
 177     0.80  0.61   0.14          0.93  1.47    0.48  0.80    2.29  1.69

  152       0.01     DIBUTYLPHTHALATE   84742
  57     0.29  0.23   0.05          0.34  0.52    0.19  0.31    0.68  0.48
 149     7.17  5.52   1.33          8.27 12.80    4.55  7.54   16.55 11.80
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              Internal/External Standard File for Cmpd Class # 6

   Cmpd#     Recovery    Compound Name
               Std #59     Std #60       Std #61       Std #62        Std #63
   Mass     110   125     82    110    264     -       188     -       99     -


    140       0.01      N-NONADECANE       629925
     71     1.51  5.27   2.24  0.87   0.68             0.16            2.35
     85     1.01  3.47   1.50  0.58   0.45             0.11            1.57

    141       0.01      N-EICOSANE 1112958
     57     3.08 10.35   4.25  1.63   1.57             0.35            4.63
     71     2.11  7.09   2.91  1.12   1.07             0.23            3.17

    142       0.01      N-HENEICOSANE  629947
     57     2.73  9.53   4.11  1.60   1.07             0.30            4.31
     71     1.89  6.60   2.85  1.10   0.74             0.21            2.99

    143       0.01      N-DOCOSANE 629970
     57     2.89  9.60   4.14  1.60   1.22             0.30            4.35
     71     2.02  6.71   2.89  1.12   0.85             0.21            3.04

    144       0.01      N-TRICOSANE  638675
     57     3.10 10.28   4.42  1.71   1.29             0.32            4.65
     71     2.18  7.22   3.11  1.20   0.90             0.22            3.27

    145       0.01      PHENYLACETATE    122792
     94     1.31  4.43   1.72  0.67   0.70             0.13            1.98
    136     0.18  0.62   0.24  0.09   0.10             0.02            0.28

    146       0.01      BENZYLACETATE     140114
     91     0.38  1.25   0.48  0.19   0.20             0.04            0.56
    108     0.79  2.63   1.02  0.40   0.41             0.07            1.17

    147       0.01      METHYLBENZENESULFONATE
     77     0.91  3.04   1.31  0.51   0.40             0.09            1.38
    172     0.32  1.08   0.47  0.18   0.14             0.03            0.49

    148       0.01      METHYLTOLUENESULFONATE(P)
     91     1.17  3.90   1.68  0.65   0.51             0.12            1.76
    155     0.52  1.74   0.75  0.29   0.23             0.05            0.79

    149       0.01      DIMETHYLPHTHALATE      131113
     77     0.57  1.83   0.75  0.29   0.28             0.06            0.85
    163     3.68 11.87   4.88  1.88   1.85             0.41            5.51

    150       0.01      ETHYLTOLUENESULFONATE(P)  80400
     91     1.28  4.25   1.83  0.71   0.55             0.13            1.92
    155     0.91  3.01   1.30  0.50   0.38             0.09            1.36

    151       0.01      DIETHYLPHTHALATE 84662
    149     2.35  7.82   3.34  1.30   1.02             0.24            3.54
    177     0.59  1.97   0.85  0.33   0.26             0.06            0.89

    152       0.01      DIBUTYLPHTHALATE   84742
     57     0.20  0.68   0.28  0.11   0.10             0.02            0.31
    149     4.99 16.75   6.88  2.64   2.52             0.55            7.47
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         Internal/External Standard File for Cmpd Class # 6

Cmpd#     Recovery    Compound Name
            Std # 2      Std #54        Std #56        Std #57        Std #58
Mass      109   236    136    -       82   128       98   116       84   112


 153       0.01       BUTYLBENZYLPHTHALATE
  91     2.09  1.62    0.38           2.28  3.69    1.48  2.48     4.64  3.41
 149     3.37  2.62    0.62           3.69  5.95    2.40  4.01     7.49  5.51

 154       0.01       DIETHYLHEXYLPHTHALATE 117817
 149     5.22  4.07    0.96           5.71  9.23    3.74  6.26    11.59  8.53
 167     1.98  1.54    0.37           2.17  3.51    1.42  2.37     4.40  3.24

 155       0.01       BENZALDEHYDE     100527
  77     0.36  0.28    0.07           0.42  0.64    0.23  0.38     0.84  0.60
 105     0.40  0.31    0.07           0.46  0.70    0.25  0.42     0.92  0.66

 156       0.01       TOLUALDEHYDE(P)     529204
  91     0.54  0.44    0.10           0.65  1.04    0.34  0.57     1.65  1.21
 119     0.63  0.51    0.12           0.77  1.23    0.41  0.68     1.95  1.43

 157       0.01       ACETOPHENONE      98862
  77     0.38  0.64    0.15           0.96  1.53    0.53  0.87     1.93  1.37
 105     1.22  0.94    0.23           1.41  2.25    0.78  1.29     2.85  2.03

 158       0.01       SALICYLALDEHYDE     90028
 121     0.56  0.44    0.10           0.61  0.99    0.40  0.67     1.24  0.91
 122     0.60  0.47    0.11           0.60  1.07    0.43  0.72     1.34  0.99

 159       0.01       ANISALDEHYDE      123115
 135     1.37  1.08    0.25           1.53  2.47    0.91  1.66     3.11  2.29
 136     0.96  0.76    0.18           1.07  1.73    0.70  1.16     2.18  1.60

 160       0.01       PHENOL 108952
  94     1.07  0.84    0.20           1.18  1.90    0.76  1.27     2.41  1.77

 161       0.01       CRESOL(P)  106445
 107     1.21  0.93    0.23           1.40  2.25    0.80  1.29     2.91  2.08
 108     1.07  0.82    0.20           1.24  1.99    0.69  1.14     2.58  1.84

 162       0.01       2,3-DIMETHYLPHENOL   526750
 107     0.87  0.67    0.16           1.00  1.61    0.57  0.95     2.08  1.48
 122     0.91  0.70    0.17           1.05  1.64    0.58  0.96     2.12  1.51

 163       0.01       ISOPROPYLPHENOL     88699
 121     1.79  1.36    0.32           2.04  3.25    1.07  1.78     5.10  3.77
 136     0.07  0.56    0.12           0.75  1.19    0.39  0.65     1.87  1.38

 164       0.01       O-NITROPHENOL  88755
  65     0.03  0.02    0.00           0.03  0.05    0.02  0.03     0.06  0.05
 139     0.13  0.10    0.02           0.14  0.23    0.09  0.15     0.29  0.21

 165       0.01       4-CHLORO-3-METHYLPHENOL 59507
 107     0.93  0.71    0.17           1.06  1.68    0.55  0.92     2.64  2.95
 142     1.02  0.77    0.18           1.16  1.84    0.61  1.01     2.89  2.14
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          Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std #59     Std #60      Std #61      Std #62      Std #63
Mass     110   125    82   110     264    -     188    -      99    -


 153       0.01     BUTYLBENZYLPHTHALATE
  91    1.51  5.02   1.95  0.76   0.78           0.14          2.24
 149    2.44  8.10   3.15  1.22   1.26           0.23          3.62

 154       0.01     DIETHYLHEXYLPHTHALATE 117817
 149    4.03 12.58   4.88  1.89   1.90           0.35          5.61
 167    1.53  4.78   1.85  0.72   0.72           0.13          2.13

 155       0.01     BENZALDEHYDE    100527
  77    0.25  0.84   0.35  0.13   0.13           0.03          0.38
 105    0.28  0.93   0.38  0.15   0.14           0.03          0.42

 156       0.01     TOLUALDEHYDE(P)    529204
  91    0.42  1.41   0.61  0.24   0.15           0.05          0.64
 119    0.50  1.66   0.72  0.28   0.22           0.05          0.75

 157       0.01     ACETOPHENONE     98862
  77    0.57  1.95   0.80  0.31   0.29           0.06          0.87
 105    0.85  2.88   1.18  0.45   0.43           0.09          1.28

 158       0.01     SALICYLALDEHYDE    90028
 121    0.41  1.35   0.52  0.20   0.21           0.04          0.60
 122    0.44  1.46   0.56  0.22   0.23           0.04          0.65

 159       0.01     ANISALDEHYDE     123115
 135    1.01  3.36   1.30  0.51   0.53           0.09          1.50
 136    0.71  2.36   0.91  0.35   0.37           0.07          1.05

 160       0.01     PHENOL 108952
  94    0.75  2.60   1.01  0.39   0.41           0.07          1.15

 161       0.01     CRESOL(P)  106445
 107    0.88  2.85   1.17  0.45   0.44           0.10          1.31
 108    0.78  2.52   1.03  0.40   0.39           0.09          1.16

 162       0.01     2,3-DIMETHYLPHENOL   526750
 107    0.63  2.11   0.84  0.32   0.32           0.07          0.94
 122    0.64  2.14   0.85  0.33   0.32           0.07          0.95

 163       0.01     ISOPROPYLPHENOL    88699
 121    1.28  4.39   1.90  0.73   0.58           0.14          1.99
 136    0.47  1.61   0.69  0.27   0.21           0.05          0.73

 164       0.01     O-NITROPHENOL  88755
  65    0.02  0.07   0.03  0.01   0.01           0.00          0.03
 139    0.09  0.31   0.12  0.05   0.05           0.01          0.14

 165       0.01     4-CHLORO-3-METHYLPHENOL 59507
 107    0.66  2.27   0.98  0.38   0.30           0.07          1.03
 142    0.72  2.49   1.07  0.42   0.32           0.08          1.13
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                  Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56        Std #57        Std #58
Mass     109   236   136     -       82    128      98   116       84   112


 166       0.01     4-CHLOROCRESOL
 107     0.83  0.64   0.16         0.97  1.57    0.53  0.88     2.03  1.45
 142     0.94  0.72   0.17         1.09  1.77    0.60  0.99     2.29  1.63

 167       0.01     1-NAPHTHOL         90153
 115     0.35  0.26   0.06         0.38  0.61    0.20  0.34     0.96  0.72
 144     0.61  0.45   0.11         0.67  1.07    0.35  0.29     1.68  1.25

 168       0.01     P-TERT-BUTYLPHENOL  98544
 107     0.56  0.43   0.10         0.65  1.03    0.34  0.56     1.60  1.18
 135     1.96  1.49   0.35         2.22  3.54    1.17  1.94     5.56  4.11

 169       0.01     2-NITROCRESOL  119335
  77     0.26  0.20   0.05         0.30  0.46    0.07  0.27     0.60  0.43
 153     0.74  0.57   0.14         0.83  1.33    0.46  0.78     1.72  1.23

 170       0.01     2,4-DICHLOROPHENOL   120832
 162     1.13  0.88   0.21         1.24  2.00    0.80  1.34     2.52  1.86
 164     0.72  0.53   0.13         0.78  1.27    0.51  0.85     1.60  1.18

 171       0.01     2,4,6-TRICHLOROPHENOL 88062
 196     0.81  0.63   0.15         0.89  1.44    0.58  0.97     1.88  1.34
 198     0.83  0.64   0.15         0.91  1.46    0.59  0.98     1.90  1.36

 172       0.01     DI-TERT-BUTYL-4-METHYLPHENOL      128370
 205     2.53  1.97   0.47         2.78  4.49    1.81  3.03     5.66  4.16
 220     0.67  0.52   0.12         0.73  1.18    0.48  0.80     1.49  1.09

 173       0.01     PENTACHLOROPHENOL 87865
 264     0.29  0.22   0.05         0.34  0.54    0.19  0.31     0.72  0.52
 266     0.47  0.36   0.09         0.55  0.91    0.32  0.54     1.17  0.84

 174       0.01     2-METHYLNAPHTHALENE   83329
 141     2.03  1.58   0.38         2.23  3.60    1.44  2.42     4.53  3.34
 142     2.51  1.96   0.46         2.76  4.45    1.79  2.99     5.62  4.13

 175       0.01     ACENAPHTHENE   83329
 153     1.26  0.98   0.23         1.38  2.22    0.89  1.49     2.81  2.06
 154     3.40  2.64   0.63         3.73  6.02    2.41  4.04     7.59  5.58

 176       0.01     BIPHENYL  92524
 154     2.28  1.78   0.42         2.51  4.04    1.63  2.72     5.10  3.75

 177       0.01     1,8-DIMETHYLNAPHTHALENE     569415
 141     1.59  1.24   0.29         1.74  2.82    1.13  1.89     3.55  2.61
 156     2.30  1.79   0.42         2.52  4.07    1.63  2.73     5.13  3.77

 178       0.01     FLUORENE  86737
 165     2.74  2.13   0.49         3.01  4.85    1.95  3.27     6.12  4.50
 166     3.07  2.38   0.57         3.44  5.55    2.23  3.74     6.99  5.14
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              Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery    Compound Name
          Std #59      Std #60      Std #61       Std #62       Std #63
Mass     110   125     82   110     264    -      188    -      99    -


 166       0.01      4-CHLOROCRESOL
 107     0.58  1.96    0.80  0.31    0.31          0.07          0.91
 142     0.66  2.20    0.85  0.34    0.35          0.08          1.03

 167       0.01      1-NAPHTHOL          90153
 115     0.25  0.83    0.36  0.14    0.11          0.03          0.38
 144     0.44  1.45    0.62  0.24    0.18          0.05          0.66

 168       0.01      P-TERT-BUTYLPHENOL  98544
 107     0.40  1.38    0.66  0.23    0.18          0.04          0.62
 135     1.44  4.79    2.04  0.80    0.63          0.15          2.16

 169       0.01      2-NITROCRESOL  119335
  77     0.18  0.61    0.25  0.10    0.09          0.02          0.27
 153     0.52  1.74    0.71  0.27    0.26          0.06          0.78

 170       0.01      2,4-DICHLOROPHENOL   120832
 162     0.80  2.73    1.05  0.41    0.43          0.08          1.22
 164     0.51  1.70    0.67  0.26    0.27          0.05          0.77

 171       0.01      2,4,6-TRICHLOROPHENOL 88062
 196     0.58  1.97    0.76  0.30    0.91          0.05          0.88
 198     0.58  1.99    0.77  0.30    0.32          0.06          0.89

 172       0.01      DI-TERT-BUTYL-4-METHYLPHENOL       128370
 205     1.85  6.13    2.37  0.92    0.96          0.17          2.73
 220     0.49  1.61    0.62  0.24    0.25          0.05          0.72

 173       0.01      PENTACHLOROPHENOL 87865
 264     0.20  0.68    0.28  0.11    0.11          0.02          0.31
 266     0.36  1.11    0.45  0.07    0.18          0.04          0.50

 174       0.01      2-METHYLNAPHTHALENE   83329
 141     1.48  4.91    1.90  0.74    0.77          0.14          2.19
 142     1.78  6.08    2.36  0.91    0.95          0.17          2.71

 175       0.01      ACENAPHTHENE   83329
 153     0.92  3.04    1.18  0.46    0.47          0.09          1.35
 154     2.48  8.22    3.19  1.23    1.28          0.23          3.66

 176       0.01      BIPHENYL  92524
 154     1.67  5.52    2.14  0.83    0.87          0.16          2.46

 177       0.01      1,8-DIMETHYLNAPHTHALENE     569415
 141     1.16  3.84    1.49  0.58    0.60          0.11          1.71
 156     1.67  5.55    2.15  0.83    0.87          0.16          2.48

 178       0.01      FLUORENE  86737
 165     2.00  6.62    2.57  0.99    1.04          0.19          2.95
 166     2.28  7.57    2.93  1.14    1.19          0.21          3.38
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           Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54        Std #56       Std #57       Std #58
Mass     109   236    136    -       82   128      98   116      84   112


 179       0.01      2,3,5-TRIMETHYLNAPHTHALENE   2245387
 155    1.86  1.44    0.34           2.08  3.36    1.36  2.27    4.24  3.12
 170    2.56  1.99    0.47           2.86  4.62    1.86  3.11    5.83  4.29

 180       0.01      ANTHRACENE  120127
 178    3.21  2.47    0.60           3.71  5.74    2.04  3.38    7.43  5.30

 181       0.01      PYRENE    129000
 202    4.88  3.75    0.95           5.66  8.73    3.27  5.18   11.54  8.23

 182       0.01      9,10-DIMETHYLANTHRACENE   781431
 191    1.33  1.03    0.25           1.45  2.35    0.94  1.57    2.96  2.18
 206    2.85  2.22    0.53           3.13  5.04    2.01  3.37    6.36  4.68

 183       0.01      CHRYSENE        218019
 228    2.21  1.73    0.41           2.42  3.92    1.59  2.66    4.91  3.61

 184       0.01      PERYLENE   198550
 252    1.60  1.23    0.30           1.84  2.86    1.02  1.68    3.67  2.62

 185       0.01      DICYANOBUTANE     111693
  41    0.66  0.51    0.12           0.72  1.17    0.47  0.79    1.47  1.08
  54    0.29  0.23    0.05           0.32  0.52    2.10  0.35    0.66  0.48

 186       0.01      BUTYLCARBAMATE  14994775
  41    0.48  0.36    0.08           0.54  0.86    0.28  0.47    1.35  1.00
  59    0.24  0.26    0.05           0.29  0.47    0.15  0.25    0.72  0.54

 187       0.01      DIBUTYLDISULFIDE      110065
  41    0.73  0.56    0.13           0.84  1.34    0.44  0.73    2.10  1.55
  57    3.09  2.36    0.56           3.54  5.64    1.85  3.09    8.84  6.54

 188       0.01      BIS(2-CHLOROETHYL)ETHANE  112265
  63    1.71  1.31    0.31           1.97  3.13    1.03  1.71    4.91  3.63
  93    0.84  0.65    0.15           0.97  1.54    0.51  0.84    2.42  1.78

 189       0.01      TRIBUTYLPHOSPHATE     126738
  99    4.03  3.10    0.75           4.65  7.20    2.56  4.24    9.28  6.62
 155    0.88  0.68    0.16           1.01  1.57    0.56  0.92    2.02  1.44

 190       0.01      ALDRIN    309002
  66    1.33  1.03    0.24           1.49  2.40    0.97  1.62    3.03  2.23
 263    0.60  0.46    0.11           0.67  1.08    0.44  0.73    1.36  1.00

 191       0.01      DIHYDROBENZOFURAN      496162
  91    0.68  0.52    0.13           0.79  1.25    0.43  0.72    1.58  1.13
 120    0.97  0.75    0.18           1.12  1.67    0.66  0.78    2.16  1.54

 192       0.01      NITROBENZENE       98953
  77    0.86  0.67    0.16           0.94  1.51    0.61  1.02    1.91  1.40
 123    0.54  0.42    0.10           0.59  0.95    0.38  0.64    1.20  0.88
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              Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std #59      Std #60       Std #61        Std #62        Std #63
Mass      110   125     82   110     264     -      188     -       99     -


 179      0.01      2,3,5-TRIMETHYLNAPHTHALENE    2245387
 155   1.38  4.59    1.78  0.69    0.72            0.13            2.05
 170   1.90  6.31    2.44  0.95    0.99            0.18            2.81

 180      0.01      ANTHRACENE   120127
 178   2.24  7.59    3.08  1.19    1.13            0.25            3.35

 181      0.01      PYRENE     129000
 202   3.59 11.47    4.95  1.90    1.80            0.40            5.36

 182      0.01      9,10-DIMETHYLANTHRACENE    781431
 191   0.96  3.19    1.24  0.48    0.50            0.09            1.42
 206   2.06  6.86    2.67  1.03    1.08            0.19            3.06

 183      0.01      CHRYSENE       218019
 228   1.61  5.34    2.07  0.80    0.81            0.15            2.39

 184      0.01      PERYLENE    198550
 252   1.11  3.72    1.53  0.59    0.47            0.12            1.65

 185      0.01      DICYANOBUTANE     111693
  41   0.48  1.59    0.62  0.24    0.25            0.05            0.71
  54   0.22  0.71    0.28  0.11    0.11            0.02            0.32

 186      0.01      BUTYLCARBAMATE  14994775
  41   0.35  1.16    0.50  0.09    0.15            0.04            0.52
  59   0.19  0.63    0.27  0.11    0.08            0.02            0.28

 187      0.01      DIBUTYLDISULFIDE      110065
  41   0.54  1.78    0.78  0.31    0.20            0.06            0.82
  57   2.21  7.62    3.29  1.27    1.00            0.24            3.42

 188      0.01      BIS(2-CHLOROETHYL)ETHANE  112265
  63   1.27  4.23    1.83  0.71    0.56            0.13            1.91
  93   0.61  2.08    0.90  0.35    0.27            0.06            0.94

 189      0.01      TRIBUTYLPHOSPHATE     126738
  99   2.81  9.43    3.87  1.49    1.41            0.31            4.19
 155   0.61  2.05    0.84  0.32    0.31            0.07            0.91

 190      0.01      ALDRIN     309002
  66   0.99  3.28    1.27  0.49    0.51            0.09            1.46
 263   0.44  1.47    0.57  0.22    0.23            0.04            0.66

 191      0.01      DIHYDROBENZOFURAN      496162
  91   0.27  1.59    0.65  0.25    0.24            0.05            0.71
 120   0.68  2.27    0.90  0.35    0.33            0.07            0.98

 192      0.01      NITROBENZENE       98953
  77   0.61  2.07    0.80  0.31    0.33            0.06            0.94
 123   0.38  1.30    0.50  0.20    0.21            0.04            0.59
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         Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass      109   236    136    -      82    128     98    116     84    112


 193       0.01      BENZOTHIAZOLE        95169
 135     1.56  1.21   0.29          1.71  2.76   1.11  1.86   3.47  2.55

 194       0.01      PHENYLCARBAMATE      102090
  94     1.25  0.96   0.23          1.44  2.23   0.79  1.31   2.88  2.06
 137     0.02  0.01   0.00          0.02  0.03   0.01  0.02   0.04  0.03

 195       0.01      2,4-DINITROTOLUENE      121142
  89     0.35  0.28   0.06          0.40  0.65   0.26  0.44   0.81  0.60
 165     0.71  0.53   0.13          0.75  1.21   0.46  0.76   1.53  1.13

 196       0.01      BENZYLSULFIDE  538749
  91     3.55  2.68   0.63          4.00  6.38   2.10  3.49   9.99  7.42
 123     0.90  0.68   0.16          1.02  1.62   0.53  0.89   2.54  1.88

 197       0.01      DIPHENYLSULFONE   127639
 125     3.82  3.44   0.81          5.16  8.21   2.71  4.51  12.95  8.65
 218     0.92  0.73   0.17          1.10  1.75   0.58  0.96   2.74  2.03

 198       0.01      TRIPHENYLPHOSPHATE  115866
 325     2.59  2.01   0.13          0.79  1.28   0.52  0.87   1.61  1.18
 326     0.09  0.07   0.17          1.03  1.67   0.68  1.14   2.09  1.54

 199       0.01      DIPHENYLMERCURY   587859
  77     0.72  0.56   0.48          2.85  4.59   1.96  3.28   6.08  4.47
 356     0.95  0.74   0.02          0.09  0.15   0.06  0.11   0.20  0.15

 200       0.01      TETRAPHENYLTIN
 197     1.40  1.13   0.27          1.70  2.71   0.89  1.47   4.21  3.13
 351     1.30  1.05   0.25          1.58  2.51   0.82  1.37   3.91  2.91

 201       0.01      BENZYLCHLORIDE   100447
  91     1.55  1.18   0.28          1.77  2.82   0.93  1.54   4.42  3.28
 126     0.42  0.32   0.08          0.48  0.76   0.25  0.42   1.20  0.89

 202       0.01      4-CHLOROBENZONITRILE 623030
 102     0.55  0.42   0.10          0.63  0.99   0.33  0.55   1.57  1.16
 137     2.10  1.57   0.36          2.38  3.79   1.25  2.08   5.95  4.40

 203       0.01      3-CHLOROBENZALDEHYDE     587042
 111     0.06  0.05   0.01          0.08  0.12   0.04  0.07   0.20  0.14
 139     0.12  0.10   0.02          0.15  0.24   0.08  0.13   0.38  0.28

 204       0.01      O-CHLOROANISOLE     766518
 127     0.60  0.46   0.11          0.69  1.09   0.36  0.60   1.71  1.27
 142     1.32  1.00   0.24          0.50  2.40   0.79  1.31   3.76  2.78

 205       0.01      CHLOROBENZAMIDE  619567
 139     0.70  0.55   0.13          0.77  1.25   0.50  0.84   1.57  1.16
 155     0.38  0.30   0.07          0.42  0.68   0.27  0.46   0.85  0.63
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            Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery    Compound Name
          Std #59     Std #60     Std #61      Std #62      Std #63
Mass     110   125    82   110    264    -     188    -     99    -


 193       0.01      BENZOTHIAZOLE        95169
 135    1.14  3.76   1.46  0.57   0.59          0.11         1.68

 194       0.01      PHENYLCARBAMATE      102090
  94    0.87  2.92   1.20  0.46   0.44          0.10         1.30
 137    0.01  0.04   0.01  0.01   0.00          0.00         0.02

 195       0.01      2,4-DINITROTOLUENE      121142
  89    0.27  0.88   0.34  0.13   0.14          0.03         0.39
 165    0.50  1.66   0.64  0.25   0.26          0.05         0.74

 196       0.01      BENZYLSULFIDE  538749
  91    2.47  8.62   3.72  1.44   1.11          0.27         3.90
 123    0.63  2.19   0.94  0.37   0.28          0.07         0.99

 197       0.01      DIPHENYLSULFONE   127639
 125    3.00 11.09   4.77  1.85   1.22          0.35         5.05
 218    0.67  2.36   1.02  0.29   0.30          0.07         1.07

 198       0.01      TRIPHENYLPHOSPHATE  115866
 325    1.98  6.58   2.55  0.95   1.03          0.18         0.78
 326    0.06  0.22   0.08  0.03   0.03          0.01         1.02

 199       0.01      DIPHENYLMERCURY   587859
  77    0.53  1.75   0.68  0.26   0.26          0.05         2.94
 356    0.69  2.28   0.88  0.34   0.35          0.06         0.10

 200       0.01      TETRAPHENYLTIN
 197    1.10  3.66   1.57  0.61   0.44          0.11         1.56
 351    1.03  3.40   1.46  0.57   0.41          0.11         1.54

 201       0.01      BENZYLCHLORIDE   100447
  91    1.10  3.81   1.64  0.64   0.50          0.12         1.71
 126    0.30  1.03   0.45  0.17   0.12          0.03         0.47

 202       0.01      4-CHLOROBENZONITRILE 623030
 102    0.39  1.35   0.58  0.23   0.18          0.04         0.61
 137    1.49  5.12   2.21  0.85   0.67          0.16         2.32

 203       0.01      3-CHLOROBENZALDEHYDE     587042
 111    0.05  0.17   0.07  0.03   0.02          0.00         0.08
 139    0.10  0.32   0.14  0.05   0.04          0.01         0.15

 204       0.01      O-CHLOROANISOLE    766518
 127    0.43  1.48   0.64  0.25   0.17          0.05         0.67
 142    0.94  3.24   1.40  0.54   0.36          0.10         1.46

 205       0.01      CHLOROBENZAMIDE  619567
 139    0.51  1.70   0.66  0.26   0.27          0.05         0.76
 155    0.28  0.92   0.36  0.14   0.15          0.03         0.41
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               Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery   Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass     109   236    136     -       82   128      98   116      84   112


 206       0.01      3,4-DICHLOROBENZALDEHYDE 6287383
 173     0.48  0.39   0.09           0.58  0.93    0.31  0.57    1.46  1.07
 174     0.32  0.26   0.06           0.39  0.62    0.21  0.34    0.98  0.72

 207       0.01      1,2,4-TRICHLOROBENZENE  120821
 145     0.34  0.26   0.06           0.40  0.63    0.22  0.36    0.80  0.57
 180     1.30  1.00   0.24           1.50  2.40    0.83  1.37    3.03  2.16

 208       0.01      2-BROMO-1-CHLOROBENZENE 694804
 190     0.78  0.61   0.14           0.85  1.38    0.55  0.92    1.74  1.28
 192     1.04  0.81   0.19           1.14  1.84    0.74  1.24    2.33  1.71

 209       0.01      1,2-DICHLORONAPHTHALENE  2050693
 161     0.44  0.34   0.08           0.50  0.78    0.28  0.46    1.01  0.72
 196     2.17  1.67   0.40           2.51  3.88    1.38  2.29    5.03  3.58

 210       0.01      1,2,4,5-TETRACHLOROBENZENE  95943
 214     1.18  0.90   0.22           1.29  2.09    0.84  1.40    2.63  1.94
 216     1.54  1.18   0.28           1.69  2.72    1.09  1.83    3.43  2.52

 211       0.01      P-DIBROMOBENZENE   106376
 234     0.68  0.52   0.12           0.77  1.23    0.41  0.67    1.93  1.43
 236     1.29  1.00   0.23           1.48  2.36    0.78  1.30    3.77  2.93

 212       0.01      4-BROMODIPHENYLETHER
 248     1.08  0.81   0.20           1.19  1.92    0.77  1.29    2.42  1.78
 250     1.13  0.88   0.21           1.26  2.04    0.82  1.37    2.57  1.89

 213       0.01      HEXACHLOROBENZENE   118741
 284     0.74  0.56   0.13           0.84  1.34    0.44  0.73    2.10  1.55
 286     0.60  0.46   0.11           0.68  1.08    0.36  0.59    1.70  1.26
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              Internal/External Standard File for Cmpd Class # 6

Cmpd#    Recovery    Compound Name
          Std #59      Std #60      Std #61       Std #62       Std #63
Mass     110   125    82   110     264    -      188    -       99    -


 206       0.01      3,4-DICHLOROBENZALDEHYDE 6287383
 173    0.37  1.25    0.54  0.21    0.17          0.04          0.57
 174    0.25  0.84    0.36  0.14    0.11          0.03          0.38

 207       0.01      1,2,4-TRICHLOROBENZENE  120821
 145    0.24  0.80    0.33  0.13    0.12          0.03          0.36
 180    0.89  3.05    1.25  0.48    0.46          0.10          1.36

 208       0.01      2-BROMO-1-CHLOROBENZENE 694804
 190    0.57  1.88    0.73  0.28    0.30          0.05          0.84
 192    0.76  2.52    0.98  0.38    0.40          0.07          1.12

 209       0.01      1,2-DICHLORONAPHTHALENE  2050693
 161    0.31  1.02    0.42  0.16    0.15          0.03          0.46
 196    1.52  5.08    2.08  0.80    0.76          0.17          2.27

 210       0.01      1,2,4,5-TETRACHLOROBENZENE  95943
 214    0.86  2.85    1.11  0.43    0.45          0.08          1.27
 216    1.12  3.72    1.44  0.56    0.58          0.11          1.66

 211       0.01      P-DIBROMOBENZENE   106376
 234    0.49  1.66    0.72  0.28    0.19          0.05          0.75
 236    0.93  3.18    1.38  0.53    0.45          0.10          1.45

 212       0.01      4-BROMODIPHENYLETHER
 248    0.79  2.61    1.01  0.39    0.41          0.07          1.17
 250    0.84  2.78    1.08  0.42    0.44          0.08          1.24

 213       0.01      HEXACHLOROBENZENE   118741
 284    0.53  1.83    0.78  0.30    0.24          0.06          0.82
 286    0.43  1.46    0.63  0.24    0.19          0.05          0.66
```

Table B-7. RMRs AND RECOVERIES FOR WABN COMPOUNDS (FU, pH 8.0)

Class No. 7

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

		Standard							
		d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98	1.72(9)[a]	-	1.67(1)	.29(6)	1.79(8)	2.84(8)	4.21(22)	3.02(21)
	116	1.03(9)	.60(0)	-	.18(6)	1.07(8)	1.71(8)	2.53(22)	1.81(21)
d_8-naphthalene	136	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82	.97(4)	.57(10)	.95(10)	.16(3)	-	1.60(1)	2.35(17)	1.70(16)
	128	.61(2)	.35(9)	.59(9)	.10(1)	.63(1)	-	1.47(16)	1.07(15)
d_5-phenylethanol	84	.42(15)	.25(24)	.42(24)	.071 ~~.21~~(18)	.44(16)	.70(15)	-	.73(2)
	112	.58(15)	.35(22)	.58(23)	.098(18)	.61(16)	.95(16)	1.39(2)	-
d_5-propiophenone	82	1.09(4)	.65(13)	1.07(14)	.18(8)	1.13(6)	1.82(6)	2.63(11)	1.90(10)
	110	2.85(5)	1.67(13)	2.78(14)	.48(17)	2.94(6)	4.72(6)	6.84(12)	4.95(11)
d_5-acetophenone	110	1.52(2)	.90(7)	1.50(8)	.25(4)	1.60(5)	2.55(1)	3.71(17)	2.68(16)
	125	.46(2)	.27(8)	.45(7)	~~.36~~(3) .076	.48(3)	.76(4)	1.11(18)	.81(17)
d_{12}-perylene	264	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109	1.10(4)	.65(7)	1.08(8)	.18(3)	1.14(2)	1.82(2)	2.69(18)	1.97(19)
	236	1.43(4)	.84(6)	1.39(7)	.24(6)	1.48(3)	2.37(3)	3.48(18)	2.52(18)

(continued)

		Standard							
		d_5-Propiophenone		d_5-Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-Iodotoluene	
Compound	Ion	m/z 82	m/z 110	m/z 110	m/z 125	m/z 264	m/z 188	m/z 109	m/z 236
d_5-phenol	99	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-o-xylene	98	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

[a] (CV).

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               Internal/External Standard File for Cmpd Class # 7

Cmpd#     Recovery    Compound Name
           Std # 2      Std #54        Std #56        Std #57        Std #58
Mass      109   236     136    -       82    128      98    116      84    112


 100        0.01      PYRIDINE  110861
  52     0.29  0.22    0.05           0.33  0.51     0.19  0.32     0.67  0.48
  79     0.44  0.34    0.08           0.51  0.78     0.30  0.50     1.10  0.78

 101        0.01      ALPHA-PICOLINE      109068
  66     0.26  0.20    0.05           0.30  0.46     0.16  0.27     0.59  0.42
  93     0.66  0.51    0.12           0.76  1.18     0.40  0.66     1.52  1.09

 102        0.01      ANILINE        62533
  66     0.23  0.19    0.04           0.28  0.41     0.15  0.24     0.53  0.38
  93     0.76  0.54    0.13           0.81  1.25     0.45  0.74     1.62  1.15

 103        0.01      LUTIDINE      108485
 106     0.13  0.10    0.02           0.15  0.25     0.08  0.13     0.39  0.28
 107     0.22  0.16    0.04           0.24  0.39     0.13  0.21     0.61  0.45

 104        0.01      TOLUIDINE  106490
 106     0.89  0.69    0.16           0.97  1.57     0.64  1.07     1.97  1.45
 107     0.71  0.56    0.13           0.78  1.27     0.51  0.86     1.58  1.16

 105        0.01      INDOLE  120729
  90     0.72  0.54    0.13           0.82  1.30     0.43  0.71     2.04  1.51
 117     1.92  1.45    0.34           2.17  3.46     1.14  1.89     5.43  4.02

 106        0.01      2,3,6-TRIMETHYLPYRIDINE   1462846
 120     0.66  0.51    0.12           0.76  1.18     0.42  0.69     1.53  1.09
 121     0.90  0.69    0.17           1.03  1.61     0.55  0.91     2.08  1.49

 107        0.01      2,6-DIMETHYLANILINE 1300738
 106     0.36  0.27    0.06           0.41  0.65     0.21  0.36     1.02  0.75
 121     0.57  0.44    0.10           0.66  1.04     0.34  0.57     1.64  1.21

 108        0.01      M-CHLOROANILINE       108429
 127     1.09  0.84    0.20           1.26  1.94     0.69  1.15     2.52  1.79
 129     0.34  0.26    0.06           0.29  0.60     0.22  0.36     0.78  0.56

 109        0.01      QUINOLINE    91225
 129     1.82  1.41    0.34           1.99  3.22     1.30  2.17     4.06  2.98

 110        0.01      P-NITROANILINE   100016
  65     0.44  0.35    0.08           0.52  0.83     0.27  0.46     1.30  0.97
 138     0.56  0.45    0.11           0.67  1.07     0.35  0.58     1.68  0.22

 111        0.01      2,4-DIMETHYLQUINOLINE   1198374
 156     0.41  0.32    0.08           0.47  0.75     0.26  0.43     0.95  0.68
 157     2.01  1.54    0.37           2.31  3.59     1.27  2.11     4.64  3.31

 112        0.01      1,8-DIAMINONAPHTHALENE
 114     0.03  0.02    0.00           0.04  0.06     0.02  0.03     0.09  0.06
 141     0.05  0.04    0.01           0.06  0.01     0.03  0.05     0.14  0.11
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              Internal/External Standard File for Cmpd Class # 7

 Cmpd#    Recovery    Compound Name
           Std #59      Std #60       Std #61       Std #62       Std #63
 Mass     110   125     82   110     264    -      188    -       99    -


  100       0.01      PYRIDINE  110861
   52    0.20  0.68    0.28  0.11   0.10           0.02           0.30
   79    0.33  1.11    0.42  0.16   0.17           0.04           0.50

  101       0.01      ALPHA-PICOLINE     109068
   66    0.18  0.60    0.25  0.09   0.09           0.02           0.27
   93    0.46  1.54    0.63  0.24   0.23           0.05           0.69

  102       0.01      ANILINE          62533
   66    0.17  0.56    0.22  0.09   0.08           0.02           0.24
   93    0.49  1.64    0.67  0.26   0.24           0.05           0.73

  103       0.01      LUTIDINE     108485
  106    0.10  0.33    0.14  0.05   0.04           0.01           0.15
  107    0.16  0.52    0.23  0.09   0.06           0.02           0.24

  104       0.01      TOLUIDINE  106490
  106    0.65  2.15    0.83  0.32   0.32           0.06           0.96
  107    0.52  1.73    0.67  0.26   0.26           0.05           0.77

  105       0.01      INDOLE  120729
   90    0.51  1.75    0.76  0.29   0.23           0.05           0.79
  117    1.40  4.68    2.02  0.78   0.61           0.15           2.12

  106       0.01      2,3,6-TRIMETHYLPYRIDINE   1462846
  120    0.46  1.54    0.63  0.24   0.23           0.05           0.67
  121    0.62  2.10    0.86  0.33   0.32           0.07           0.94

  107       0.01      2,6-DIMETHYLANILINE 1300738
  106    0.26  0.88    0.38  0.15   0.11           0.03           0.40
  121    0.42  1.41    0.61  0.24   0.18           0.04           0.64

  108       0.01      M-CHLOROANILINE       108429
  127    0.76  2.55    1.05  0.40   0.38           0.98           1.14
  129    0.24  0.79    0.33  0.13   0.12           0.03           0.35

  109       0.01      QUINOLINE    91225
  129    1.33  4.40    1.70  0.66   0.69           0.12           1.96

  110       0.01      P-NITROANILINE   100016
   65    0.34  1.13    0.49  0.19   0.14           0.04           0.51
  138    0.43  1.84    0.62  0.24   0.19           0.05           0.65

  111       0.01      2,4-DIMETHYLQUINOLINE   1198374
  156    0.29  0.96    0.40  0.15   0.15           0.03           0.43
  157    1.46  4.69    1.93  0.74   0.71           0.15           2.09

  112       0.01      1,8-DIAMINONAPHTHALENE
  114    0.02  0.08    0.03  0.01   0.01           0.00           0.03
  141    0.04  0.12    0.05  0.02   0.01           0.00           0.55
```

```
          Internal/External Standard File for Cmpd Class # 7

Cmpd#   Recovery   Compound Name
         Std # 2      Std #54      Std #56      Std #57      Std #58
Mass    109   236    136     -     82   128     98   116     84   112


  113     0.01     NICOTINE      54115
  84   1.17  0.90   0.22         1.35  2.09   0.74  1.23   2.70  1.92
 133   0.28  0.21   0.05         0.32  0.49   0.17  0.29   0.63  0.45

  114     0.01     CARBAZOLE      86748
 167   3.73  2.88   0.69         4.30  6.66   2.37  3.92   9.36  6.67

  115     0.01     2-AMINOBIPHENYL      90445
 168   6.79  5.11   1.20         7.65 12.18   4.61  6.67  19.13 14.17
 169  12.72  9.45   2.22        14.15 22.54   7.42 12.30  35.40 26.19

  116     0.01     DIPHENYLAMINE      122394
 168   1.48  1.14   0.27         1.71  2.65   0.94  1.56   3.43  2.45
 169   2.79  2.15   0.52         3.22  4.99   1.77  2.93   6.45  4.60

  117     0.01     DICYCLOHEXYLAMINE       101837
  56   0.33  0.37   0.06         0.39  0.63   0.21  0.35   1.10  0.78
 138   0.96  0.76   0.18         1.12  1.80   0.61  1.02   3.15  2.25

  118     0.01     TRIBUTYLAMINE       102829
 100   0.42  0.33   0.08         0.49  0.75   0.27  0.44   0.97  0.69
 142   1.53  1.18   0.28         1.77  2.74   0.97  1.61   3.52  2.51

  119     0.01     CAFFEINE       58082
 109   0.10  0.08   0.02         0.12  0.17   0.06  0.10   0.23  0.16
 194   0.19  0.15   0.04         0.22  0.34   0.12  0.20   0.44  0.32

  120     0.01     DIBENZYLAMINE  103491
  91   1.62  1.26   0.30         1.78  2.87   1.16  1.94   3.63  2.67
 197   0.13  0.11   0.03         0.15  0.24   0.10  0.16   0.30  0.22

  121     0.01     N,N-DIMETHYLDODECYLAMINE  112185
  58   4.72  3.88   0.87         5.47  8.83   3.58  5.99  11.09  8.16
  59   0.17  0.13   0.03         0.20  0.30   0.13  0.21   0.40  0.29

  122     0.01     ATRAZINE    1912249
 200   2.75  2.20   0.52         3.28  5.23   1.72  2.86   8.17  6.09
 215   1.67  1.34   0.31         2.00  3.18   1.05  1.74   4.97  3.71

  123     0.01     HEPTANONE(2)   110430
  43   1.21  0.94   0.22         1.33  2.14   0.85  1.14   2.32  2.00
  58   0.75  0.58   0.14         0.83  1.33   0.53  0.88   1.69  1.25

  124     0.01     BUTOXYETHANOL       111762
  41   0.21  0.17   0.04         0.25  0.40   0.13  0.22   0.49  0.35
  57   0.55  0.42   0.10         0.63  1.03   0.35  0.58   1.27  0.91

  125     0.01     2-OCTANONE    111137
  43   1.30  1.01   0.24         1.43  2.31   0.91  1.53   2.92  2.15
  58   1.02  0.79   0.19         1.11  1.80   0.71  1.19   2.27  1.67
```

```
             Internal/External Standard File for Cmpd Class # 7

Cmpd#  Recovery  Compound Name
        Std #59     Std #60     Std #61     Std #62     Std #63
Mass   110  125     82  110    264     -   188     -    99     -


  113    0.01     NICOTINE    54115
   84 0.82  2.74   1.12  0.43  0.41        0.09        1.22
  133 0.19  0.64   0.26  0.10  0.10        0.02        0.29

  114    0.01     CARBAZOLE    86748
  167 2.60  8.72   3.57  1.37  1.28        0.31        4.22

  115    0.01     2-AMINOBIPHENYL      90445
  168 4.75 16.46   7.10  2.75  2.13        0.51        7.45
  169 8.82 30.44  13.14  5.08  3.96        0.95       13.80

  116    0.01     DIPHENYLAMINE     122394
  168 1.03  3.47   1.42  0.55  0.52        0.11        1.55
  169 1.94  6.46   2.68  1.03  0.98        0.22        2.91

  117    0.01     DICYCLOHEXYLAMINE     101837
   56 0.25  0.81   0.33  0.14  0.09        0.03        0.38
  138 0.71  2.34   0.95  0.40  0.26        0.08        1.09

  118    0.01     TRIBUTYLAMINE      102829
  100 0.29  0.99   0.41  0.16  0.15        0.03        0.44
  142 0.99  3.34   1.47  0.57  0.53        0.12        1.59

  119    0.01     CAFFEINE     58082
  109 0.07  0.23   0.09  0.04  0.04        0.01        0.10
  194 0.13  0.45   0.18  0.07  0.07        0.02        0.21

  120    0.01     DIBENZYLAMINE  103491
   91 1.18  3.91   1.52  0.59  0.62        0.11        1.74
  197 0.10  0.32   0.13  0.05  0.05        0.01        0.14

  121    0.01     N,N-DIMETHYLDODECYLAMINE  112185
   58 3.62 12.02   4.66  1.81  1.87        0.34        5.37
   59 0.13  0.43   0.17  0.06  0.07        0.01        0.19

  122    0.01     ATRAZINE    1912249
  200 2.13  7.07   3.05  1.18  0.90        0.22        3.26
  215 1.21  4.30   1.85  0.72  0.55        0.13        1.95

  123    0.01     HEPTANONE(2)   110430
   43 0.88  2.91   1.13  0.44  0.47        0.08        1.30
   58 0.55  1.82   0.71  0.27  0.29        0.05        0.81

  124    0.01     BUTOXYETHANOL      111762
   41 0.15  0.49   0.20  0.09  0.07        0.02        0.22
   57 0.38  1.28   0.52  0.20  0.19        0.04        0.57

  125    0.01     2-OCTANONE    111137
   43 0.95  3.14   1.22  0.47  0.51        0.09        1.40
   58 0.74  2.45   0.95  0.37  0.39        0.07        1.09
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```
          Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54         Std #56        Std #57         Std #58
Mass     109   236     136     -       82    128      98    116       84    112


 126       0.01      BUTYLPROPIONATE   590012
  57     1.48  1.14   0.27          1.71  2.73     0.90  1.49     4.27  3.15
  75     0.44  0.34   0.08          0.51  0.82     0.27  0.45     1.28  0.95

 127       0.01      ISOPHORONE  78591
  82     1.77  1.36   0.33          2.04  3.17     1.13  1.86     4.11  2.93
 138     0.39  0.30   0.07          0.45  0.72     0.25  0.41     0.90  0.64

 128       0.01      FENCHONE   1195759
  69     0.66  0.51   0.12          0.72  1.17     0.47  0.78     1.47  1.08
  81     1.44  1.12   0.27          1.58  2.55     1.02  1.71     3.22  2.36

 129       0.01      ALPHA-TERPINEOL   98555
  59     0.56  0.43   0.10          0.65  1.00     0.36  0.59     1.31  0.93
 136     0.32  0.25   0.06          0.37  0.58     0.21  0.34     0.75  0.53

 130       0.01      N-DECANOL  112301
  41     0.40  0.31   0.07          0.46  0.74     0.25  0.42     0.92  0.66
  43     0.44  0.34   0.08          0.51  0.79     0.28  0.46     1.02  0.73

 131       0.01      DIMETHYLADIPATE  627930
  59     0.56  0.45   0.10          0.64  1.03     0.41  0.69     1.29  0.95
 114     0.44  0.35   0.08          0.49  0.79     0.32  0.54     1.00  0.74

 132       0.01      N-DECANE  124185
  43     1.47  1.11   0.26          1.67  2.66     0.88  1.46     4.18  3.09
  57     1.42  1.08   0.25          1.64  2.61     0.85  1.41     4.05  3.00

 133       0.01      N-TRIDECANE       629505
  43     2.18  1.64   0.34          2.48  3.95     1.30  2.16     6.20  4.56
  57     2.75  2.09   0.50          3.14  5.01     1.66  2.77     7.93  5.86

 134       0.01      N-TETRADECANE          629594
  43     2.52  1.92   0.45          2.88  4.58     1.51  2.51     7.19  5.31
  57     3.40  2.55   0.61          3.87  6.16     2.03  3.37     9.67  7.15

 135       0.01      N-PENTADECANE     692629
  57     2.78  2.14   0.52          3.22  4.99     1.77  2.94     6.47  4.62
  71     1.73  1.33   0.32          2.01  3.11     1.10  1.83     4.03  2.87

 136       0.01      N-HEXADECANE          544763
  43     1.90  1.45   0.34          2.16  3.45     1.13  1.89     5.41  3.99
  57     2.72  2.08   0.49          3.11  4.96     1.63  2.71     7.78  5.74

 137       0.01      N-HEPTADECANE     629787
  57     3.13  2.41   0.58          3.61  5.59     1.99  3.30     7.25  5.17
  71     2.07  1.60   0.38          2.39  3.70     1.32  2.18     4.80  3.42

 138       0.01      N-OCTADECANE   593453
  57     2.99  2.51   0.59          3.75  5.98     1.88  3.14     8.96  6.63
  71     1.98  1.66   0.39          2.48  3.95     1.25  2.08     5.95  4.41
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                Internal/External Standard File for Cmpd Class # 7

      Cmpd#    Recovery    Compound Name
                Std #59      Std #60      Std #61       Std #62       Std #63
      Mass     110   125    82   110     264    -      188    -       99    -


       126       0.01      BUTYLPROPIONATE   590012
        57    1.11  3.69    1.59  0.61    0.48            0.12          1.66
        75    0.33  1.11    0.48  0.19    0.15            0.04          0.50

       127       0.01      ISOPHORONE  78591
        82    1.23  4.14    1.70  0.65    0.62            0.14          1.80
       138    0.27  0.91    0.37  0.14    0.14            0.03          0.41

       128       0.01      FENCHONE   1195759
        69    0.48  1.58    0.62  0.24    0.25            0.05          0.71
        81    1.05  3.45    1.35  0.52    0.55            0.10          1.55

       129       0.01      ALPHA-TERPINEOL   98555
        59    0.39  1.31    0.54  0.21    0.20            0.04          0.58
       136    0.23  0.76    0.31  0.12    0.11            0.03          0.34

       130       0.01      N-DECANOL  112301
        41    0.28  0.93    0.38  0.15    0.14            0.03          0.41
        43    0.31  1.63    0.42  0.16    0.15            0.03          0.46

       131       0.01      DIMETHYLADIPATE  627930
        59    0.42  1.40    0.54  0.21    0.22            0.04          0.62
       114    0.33  1.08    0.42  0.16    0.17            0.03          0.48

       132       0.01      N-DECANE  124185
        43    1.05  3.59    1.55  0.60    0.47            0.11          1.62
        57    1.01  3.48    1.50  0.58    0.46            0.11          1.58

       133       0.01      N-TRIDECANE       629505
        43    1.56  5.33    2.30  0.89    0.70            0.17          2.41
        57    1.99  6.75    2.94  1.14    0.76            0.21          3.09

       134       0.01      N-TETRADECANE          629594
        43    1.86  6.19    2.67  1.03    0.80            0.19          2.80
        57    2.50  8.33    3.57  1.39    1.08            0.26          3.77

       135       0.01      N-PENTADECANE     692629
        57    1.94  6.52    2.68  1.03    0.99            0.22          2.92
        71    1.21  4.06    1.67  0.64    0.62            0.14          1.82

       136       0.01      N-HEXADECANE        544763
        43    1.40  4.66    2.01  0.78    0.61            0.15          2.11
        57    2.01  6.70    2.88  1.12    0.87            0.21          3.03

       137       0.01      N-HEPTADECANE     629787
        57    2.18  7.32    3.01  1.16    1.11            0.24          3.27
        71    1.44  4.85    1.99  0.77    0.73            0.16          2.17

       138       0.01      N-OCTADECANE    593453
        57    2.33  8.10    3.48  1.35    1.01            0.24          3.65
        71    1.55  5.35    2.30  0.89    0.58            0.06          2.41
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```
            Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #58
Mass     109   236    136     -      82   128      98   116      84   112


 139       0.01      N-NONADECANE  629925
  71    2.12  1.61    0.38         2.42  3.85    1.27  2.11    6.04  4.47
  85    1.42  1.08    0.25         1.61  2.57    0.85  1.41    4.03  2.98

 140       0.01      N-EICOSANE    1112958
  57    4.43  3.41    0.82         5.11  7.92    2.82  4.66   10.26  7.32
  71    3.03  2.33    0.56         3.50  5.43    1.93  3.19    7.03  5.01

 141       0.01      N-HENEICOSANE       629947
  57    3.93  2.96    0.70         4.43  7.05    2.32  3.86   11.05  8.20
  71    2.71  2.05    0.48         3.07  4.88    1.61  2.67    7.65  5.68

 142       0.01      N-DOCOSANE      629970
  57    3.73  2.98    0.70         4.46  7.10    2.33  3.88   11.11  8.26
  71    2.60  2.08    0.49         3.11  4.96    1.63  2.70    7.76  5.77

 143       0.01      N-TRICOSANE       638675
  57    3.99  3.19    0.75         4.77  7.60    2.49  4.14   11.85  8.83
  71    2.80  2.24    0.53         3.35  5.34    1.75  2.91    8.33  6.20

 144       0.01      PHENYLACETATE      122792
  94    1.84  1.43    0.34         2.01  3.25    1.30  2.18    4.10  3.01
 136    0.25  0.20    0.05         0.28  0.45    0.18  0.30    0.57  0.42

 145       0.01      BENZYLACETATE      140114
  91    0.52  0.40    0.09         0.57  0.92    0.37  0.62    1.15  0.85
 108    1.09  0.85    0.20         1.19  1.92    0.77  1.29    2.43  1.79

 146       0.01      METHYLBENZENESULFONATE
  77    1.24  0.94    0.22         1.41  2.25    0.74  1.23    3.54  2.61
 172    0.44  0.34    0.08         0.50  0.80    0.26  0.44    1.26  0.93

 147       0.01      METHYLTOLUENESULFONATE
  91    1.60  1.21    0.29         1.81  2.89    0.95  1.58    4.53  3.35
 155    0.72  0.54    0.13         0.81  1.29    0.42  0.71    2.02  1.50

 148       0.01      DIMETHYLPHTHALATE   131113
  77    0.81  0.63    0.15         0.94  1.45    0.52  0.85    1.88  1.34
 163    5.29  4.07    0.98         6.10  9.46    3.36  5.56   12.22  8.71

 149       0.01      ETHYLTOLUENESULFONATE
  91    1.74  1.32    0.31         1.97  3.14    1.03  1.72    4.92  3.65
 155    1.18  0.94    0.22         1.40  2.23    0.73  1.21    3.46  2.35

 150       0.01      DIETHYLPHTHALATE     84662
 149    3.19  2.43    0.57         3.65  5.79    1.90  3.17    9.08  6.71
 177    0.80  0.61    0.14         0.93  1.47    0.48  0.80    2.29  1.69

 151       0.01      DIBUTYLPHTHALATE     84742
  57    0.29  0.23    0.05         0.34  0.52    0.19  0.31    0.68  0.48
 149    7.17  5.52    1.33         8.27 12.80    4.55  7.54   16.55 11.80
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```
          Internal/External Standard File for Cmpd Class # 7

Cmpd#     Recovery    Compound Name
           Std #59      Std #60      Std #61       Std #62       Std #63
Mass      110   125    82   110     264    -      188    -       99    -


 139        0.01      N-NONADECANE  629925
  71     1.51  5.27   2.24  0.87   0.68           0.16          2.35
  85     1.01  3.47   1.50  0.58   0.45           0.11          1.57

 140        0.01      N-EICOSANE    1112958
  57     3.08 10.35   4.25  1.63   1.57           0.35          4.63
  71     2.11  7.09   2.91  1.12   1.07           0.23          3.17

 141        0.01      N-HENEICOSANE        629947
  57     2.73  9.53   4.11  1.60   1.07           0.30          4.31
  71     1.89  6.60   2.85  1.10   0.74           0.21          2.99

 142        0.01      N-DOCOSANE       629970
  57     2.89  9.60   4.14  1.60   1.22           0.30          4.35
  71     2.02  6.71   2.89  1.12   0.85           0.21          3.04

 143        0.01      N-TRICOSANE      638675
  57     3.10 10.28   4.42  1.71   1.29           0.32          4.65
  71     2.18  7.22   3.11  1.20   0.90           0.22          3.27

 144        0.01      PHENYLACETATE      122792
  94     1.31  4.43   1.72  0.67   0.70           0.13          1.98
 136     0.18  0.62   0.24  0.09   0.10           0.02          0.28

 145        0.01      BENZYLACETATE      140114
  91     0.38  1.25   0.48  0.19   0.20           0.04          0.56
 108     0.79  2.63   1.02  0.40   0.41           0.07          1.17

 146        0.01      METHYLBENZENESULFONATE
  77     0.91  3.04   1.31  0.51   0.40           0.09          1.38
 172     0.32  1.08   0.47  0.18   0.14           0.03          0.49

 147        0.01      METHYLTOLUENESULFONATE
  91     1.17  3.90   1.68  0.65   0.51           0.12          1.76
 155     0.52  1.74   0.75  0.29   0.23           0.05          0.79

 148        0.01      DIMETHYLPHTHALATE  131113
  77     0.57  1.83   0.75  0.29   0.28           0.06          0.85
 163     3.68 11.87   4.88  1.88   1.85           0.41          5.51

 149        0.01      ETHYLTOLUENESULFONATE
  91     1.28  4.25   1.83  0.71   0.55           0.13          1.92
 155     0.91  3.01   1.30  0.50   0.38           0.09          1.36

 150        0.01      DIETHYLPHTHALATE     84662
 149     2.35  7.82   3.34  1.30   1.02           0.24          3.54
 177     0.59  1.97   0.85  0.33   0.26           0.06          0.89

 151        0.01      DIBUTYLPHTHALATE     84742
  57     0.20  0.68   0.28  0.11   0.10           0.02          0.31
 149     4.99 16.75   6.88  2.64   2.52           0.55          7.47
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```
            Internal/External Standard File for Cmpd Class # 7

Cmpd#   Recovery   Compound Name
         Std # 2     Std #54       Std #56       Std #57       Std #58
Mass    109   236    136    -      82   128      98   116      84   112


 152      0.01     BUTYLBENZYLPHTHALATE
  91   2.09  1.62   0.38         2.28  3.69    1.48  2.48    4.64  3.41
 149   3.37  2.62   0.62         3.69  5.95    2.40  4.01    7.49  5.51

 153      0.01     DIETHYLHEXYLPHTHALATE     117817
 149   5.22  4.07   0.96         5.71  9.23    3.74  6.26   11.59  8.53
 167   1.98  1.54   0.37         2.17  3.51    1.42  2.37    4.40  3.24

 154      0.01     BENZALDEHYDE       100527
  77   0.36  0.28   0.07         0.42  0.64    0.23  0.38    0.84  0.60
 105   0.40  0.31   0.07         0.46  0.70    0.25  0.42    0.92  0.66

 155      0.01     TOLUALDEHYDE       529204
  91   0.54  0.44   0.10         0.65  1.04    0.34  0.57    1.65  1.21
 119   0.63  0.51   0.12         0.77  1.23    0.41  0.68    1.95  1.43

 156      0.01     ACETOPHENONE    98862
  77   0.38  0.64   0.15         0.96  1.53    0.53  0.87    1.93  1.37
 105   1.22  0.94   0.23         1.41  2.25    0.78  1.29    2.85  2.03

 157      0.01     SALICYLALDEHYDE   90028
 121   0.56  0.44   0.10         0.61  0.99    0.40  0.67    1.24  0.91
 122   0.60  0.47   0.11         0.60  1.07    0.43  0.72    1.34  0.99

 158      0.01     ANISALDEHYDE        123115
 135   1.37  1.08   0.25         1.53  2.47    0.91  1.66    3.11  2.29
 136   0.96  0.76   0.18         1.07  1.73    0.70  1.16    2.18  1.60

 159      0.01     PHENOL    108952
  94   1.07  0.84   0.20         1.18  1.90    0.76  1.27    2.41  1.77

 160      0.01     CRESOL(P)    106445
 107   1.21  0.93   0.23         1.40  2.25    0.80  1.29    2.91  2.08
 108   1.07  0.82   0.20         1.24  1.99    0.69  1.14    2.58  1.84

 161      0.01     2,3-DIMETHYLPHENOL      526750
 107   0.87  0.67   0.16         1.00  1.61    0.57  0.95    2.08  1.48
 122   0.91  0.70   0.17         1.05  1.64    0.58  0.96    2.12  1.51

 162      0.01     ISOPROPYLPHENOL  88699
 121   1.79  1.36   0.32         2.04  3.25    1.07  1.78    5.10  3.77
 136   0.07  0.56   0.12         0.75  1.19    0.39  0.65    1.87  1.38

 163      0.01     O-NITROPHENOL    88755
  65   0.03  0.02   0.00         0.03  0.05    0.02  0.03    0.06  0.05
 139   0.13  0.10   0.02         0.14  0.23    0.09  0.15    0.29  0.21

 164      0.01     4-CHLORO-3-METHYLPHENOL     59507
 107   0.93  0.71   0.17         1.06  1.68    0.55  0.92    2.64  2.95
 142   1.02  0.77   0.18         1.16  1.84    0.61  1.01    2.89  2.14
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              Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery    Compound Name
          Std #59      Std #60      Std #61      Std #62      Std #63
Mass     110   125     82   110     264    -     188    -      99    -


  152      0.01      BUTYLBENZYLPHTHALATE
   91    1.51  5.02   1.95  0.76   0.78         0.14          2.24
  149    2.44  8.10   3.15  1.22   1.26         0.23          3.62

  153      0.01      DIETHYLHEXYLPHTHALATE    117817
  149    4.03 12.58   4.88  1.89   1.90         0.35          5.61
  167    1.53  4.78   1.85  0.72   0.72         0.13          2.13

  154      0.01      BENZALDEHYDE       100527
   77    0.25  0.84   0.35  0.13   0.13         0.03          0.38
  105    0.28  0.93   0.38  0.15   0.14         0.03          0.42

  155      0.01      TOLUALDEHYDE       529204
   91    0.42  1.41   0.61  0.24   0.15         0.05          0.64
  119    0.50  1.66   0.72  0.28   0.22         0.05          0.75

  156      0.01      ACETOPHENONE    98862
   77    0.57  1.95   0.80  0.31   0.29         0.06          0.87
  105    0.85  2.88   1.18  0.45   0.43         0.09          1.28

  157      0.01      SALICYLALDEHYDE   90028
  121    0.41  1.35   0.52  0.20   0.21         0.04          0.60
  122    0.44  1.46   0.56  0.22   0.23         0.04          0.65

  158      0.01      ANISALDEHYDE        123115
  135    1.01  3.36   1.30  0.51   0.53         0.09          1.50
  136    0.71  2.36   0.91  0.35   0.37         0.07          1.05

  159      0.01      PHENOL    108952
   94    0.75  2.60   1.01  0.39   0.41         0.07          1.15

  160      0.01      CRESOL(P)     106445
  107    0.88  2.85   1.17  0.45   0.44         0.10          1.31
  108    0.78  2.52   1.03  0.40   0.39         0.09          1.16

  161      0.01      2,3-DIMETHYLPHENOL      526750
  107    0.63  2.11   0.84  0.32   0.32         0.07          0.94
  122    0.64  2.14   0.85  0.33   0.32         0.07          0.95

  162      0.01      ISOPROPYLPHENOL  88699
  121    1.28  4.39   1.90  0.73   0.58         0.14          1.99
  136    0.47  1.61   0.69  0.27   0.21         0.05          0.73

  163      0.01      O-NITROPHENOL     88755
   65    0.02  0.07   0.03  0.01   0.01         0.00          0.03
  139    0.09  0.31   0.12  0.05   0.05         0.01          0.14

  164      0.01      4-CHLORO-3-METHYLPHENOL     59507
  107    0.66  2.27   0.98  0.38   0.30         0.07          1.03
  142    0.72  2.49   1.07  0.42   0.32         0.08          1.13
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                 Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery     Compound Name
          Std # 2       Std #54          Std #56        Std #57        Std #58
Mass     109   236      136    -         82   128       98   116       84   112


 165       0.01       4-CHLOROCRESOL
 107     0.83  0.64     0.16            0.97  1.57     0.53  0.88     2.03  1.45
 142     0.94  0.72     0.17            1.09  1.77     0.60  0.99     2.29  1.63

 166       0.01       1-NAPHTHOL  90153
 115     0.35  0.26     0.06            0.38  0.61     0.20  0.34     0.96  0.72
 144     0.61  0.45     0.11            0.67  1.07     0.35  0.29     1.68  1.25

 167       0.01       P-TERT-BUTYLPHENOL       98544
 107     0.56  0.43     0.10            0.65  1.03     0.34  0.56     1.60  1.18
 135     1.96  1.49     0.35            2.22  3.54     1.17  1.94     5.56  4.11

 168       0.01       2-NITROCRESOL 119335
  77     0.26  0.20     0.05            0.30  0.46     0.07  0.27     0.60  0.43
 153     0.74  0.57     0.14            0.83  1.33     0.46  0.78     1.72  1.23

 169       0.01       2,4-DICHLOROPHENOL   120832
 162     1.13  0.88     0.21            1.24  2.00     0.80  1.34     2.52  1.86
 164     0.72  0.53     0.13            0.78  1.27     0.51  0.85     1.60  1.18

 170       0.01       2,4,6-TRICHLOROPHENOL  88062
 196     0.81  0.63     0.15            0.89  1.44     0.58  0.97     1.88  1.34
 198     0.83  0.64     0.15            0.91  1.46     0.59  0.98     1.90  1.36

 171       0.01       DI-TERT-BUTYL-4-METHYLPHENOL   128370
 205     2.53  1.97     0.47            2.78  4.49     1.81  3.03     5.66  4.16
 220     0.67  0.52     0.12            0.73  1.18     0.48  0.80     1.49  1.09

 172       0.01       PENTACHLOROPHENOL  87865
 264     0.29  0.22     0.05            0.34  0.54     0.19  0.31     0.72  0.52
 266     0.47  0.36     0.09            0.55  0.91     0.32  0.54     1.17  0.84

 173       0.01       2-METHYLNAPHTHALENE  91576
 141     2.03  1.58     0.38            2.23  3.60     1.44  2.42     4.53  3.34
 142     2.51  1.96     0.46            2.76  4.45     1.79  2.99     5.62  4.13

 174       0.01       ACENAPHTHENE      83329
 153     1.26  0.98     0.23            1.38  2.22     0.89  1.49     2.81  2.06
 154     3.40  2.64     0.63            3.73  6.02     2.41  4.04     7.59  5.58

 175       0.01       BIPHENYL     92524
 154     2.28  1.78     0.42            2.51  4.04     1.63  2.72     5.10  3.75

 176       0.01       1,8-DIMETHYLNAPHTHALENE  569415
 141     1.59  1.24     0.29            1.74  2.82     1.13  1.89     3.55  2.61
 156     2.30  1.79     0.42            2.52  4.07     1.63  2.73     5.13  3.77

 177       0.01       FLUORENE    86737
 165     2.74  2.13     0.49            3.01  4.85     1.95  3.27     6.12  4.50
 166     3.07  2.38     0.57            3.44  5.55     2.23  3.74     6.99  5.14
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                Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery   Compound Name
           Std #59     Std #60       Std #61        Std #62        Std #63
Mass     110   125    82   110     264     -      188     -        99     -


 165       0.01     4-CHLOROCRESOL
 107     0.58  1.96   0.80  0.31   0.31           0.07             0.91
 142     0.66  2.20   0.85  0.34   0.35           0.08             1.03

 166       0.01     1-NAPHTHOL  90153
 115     0.25  0.83   0.36  0.14   0.11           0.03             0.38
 144     0.44  1.45   0.62  0.24   0.18           0.05             0.66

 167       0.01     P-TERT-BUTYLPHENOL       98544
 107     0.40  1.38   0.66  0.23   0.18           0.04             0.62
 135     1.44  4.79   2.04  0.80   0.63           0.15             2.16

 168       0.01     2-NITROCRESOL 119335
  77     0.18  0.61   0.25  0.10   0.09           0.02             0.27
 153     0.52  1.74   0.71  0.27   0.26           0.06             0.78

 169       0.01     2,4-DICHLOROPHENOL   120832
 162     0.80  2.73   1.05  0.41   0.43           0.08             1.22
 164     0.51  1.70   0.67  0.26   0.27           0.05             0.77

 170       0.01     2,4,6-TRICHLOROPHENOL  88062
 196     0.58  1.97   0.76  0.30   0.91           0.05             0.88
 198     0.58  1.99   0.77  0.30   0.32           0.06             0.89

 171       0.01     DI-TERT-BUTYL-4-METHYLPHENOL   128370
 205     1.85  6.13   2.37  0.92   0.96           0.17             2.73
 220     0.49  1.61   0.62  0.24   0.25           0.05             0.72

 172       0.01     PENTACHLOROPHENOL  87865
 264     0.20  0.68   0.28  0.11   0.11           0.02             0.31
 266     0.36  1.11   0.45  0.07   0.18           0.04             0.50

 173       0.01     2-METHYLNAPHTHALENE  91576
 141     1.48  4.91   1.90  0.74   0.77           0.14             2.19
 142     1.78  6.08   2.36  0.91   0.95           0.17             2.71

 174       0.01     ACENAPHTHENE      83329
 153     0.92  3.04   1.18  0.46   0.47           0.09             1.35
 154     2.48  8.22   3.19  1.23   1.28           0.23             3.66

 175       0.01     BIPHENYL      92524
 154     1.67  5.52   2.14  0.83   0.87           0.16             2.46

 176       0.01     1,8-DIMETHYLNAPHTHALENE  569415
 141     1.16  3.84   1.49  0.58   0.60           0.11             1.71
 156     1.67  5.55   2.15  0.83   0.87           0.16             2.48

 177       0.01     FLUORENE    86737
 165     2.00  6.62   2.57  0.99   1.04           0.19             2.95
 166     2.28  7.57   2.93  1.14   1.19           0.21             3.38
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              Internal/External Standard File for Cmpd Class # 7

    Cmpd#    Recovery   Compound Name
              Std # 2      Std #54       Std #56      Std #57       Std #58
    Mass     109   236    136    -      82   128     98   116      84   112


     178       0.01     2,3,5-TRIMETHYLNAPHTHALENE  2245387
     155    1.86  1.44   0.34          2.08  3.36   1.36  2.27    4.24  3.12
     170    2.56  1.99   0.47          2.86  4.62   1.86  3.11    5.83  4.29

     179       0.01     ANTHRACENE      120127
     178    3.21  2.47   0.60          3.71  5.74   2.04  3.38    7.43  5.30

     180       0.01     PYRENE     129000
     202    4.88  3.75   0.95          5.66  8.73   3.27  5.18   11.54  8.23

     181       0.01     9,10-DIMETHYLANTHRACENE    781431
     191    1.33  1.03   0.25          1.45  2.35   0.94  1.57    2.96  2.18
     206    2.85  2.22   0.53          3.13  5.04   2.01  3.37    6.36  4.68

     182       0.01     CHRYSENE  218019
     228    2.21  1.73   0.41          2.42  3.92   1.59  2.66    4.91  3.61

     183       0.01     PERYLENE      198550
     252    1.60  1.23   0.30          1.84  2.86   1.02  1.68    3.67  2.62

     184       0.01     DICYANOBUTANE   111693
     41     0.66  0.51   0.12          0.72  1.17   0.47  0.79    1.47  1.08
     54     0.29  0.23   0.05          0.32  0.52   2.10  0.35    0.66  0.48

     185       0.01     BUTYLCARBAMATE  14994775
     41     0.48  0.36   0.08          0.54  0.86   0.28  0.47    1.35  1.00
     59     0.24  0.26   0.05          0.29  0.47   0.15  0.25    0.72  0.54

     186       0.01     DIBUTYLDISULFIDE 110065
     41     0.73  0.56   0.13          0.84  1.34   0.44  0.73    2.10  1.55
     57     3.09  2.36   0.56          3.54  5.64   1.85  3.09    8.84  6.54

     187       0.01     BIS(2-CHLOROETHYL)ETHANE 112265
     63     1.71  1.31   0.31          1.97  3.13   1.03  1.71    4.91  3.63
     93     0.84  0.65   0.15          0.97  1.54   0.51  0.84    2.42  1.78

     188       0.01     TRIBUTYLPHOSPHATE 126738
     99     4.03  3.10   0.75          4.65  7.20   2.56  4.24    9.28  6.62
     155    0.88  0.68   0.16          1.01  1.57   0.56  0.92    2.02  1.44

     189       0.01     ALDRIN     309002
     66     1.33  1.03   0.24          1.49  2.40   0.97  1.62    3.03  2.23
     263    0.60  0.46   0.11          0.67  1.08   0.44  0.73    1.36  1.00

     190       0.01     DIHYDROBENZOFURAN    496162
     91     0.68  0.52   0.13          0.79  1.25   0.43  0.72    1.58  1.13
     120    0.97  0.75   0.18          1.12  1.67   0.66  0.78    2.16  1.54

     191       0.01     NITROBENZENE   98953
     77     0.86  0.67   0.16          0.94  1.51   0.61  1.02    1.91  1.40
     123    0.54  0.42   0.10          0.59  0.95   0.38  0.64    1.20  0.88
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            Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery    Compound Name
          Std #59     Std #60       Std #61        Std #62        Std #63
Mass     110   125    82   110      264    -       188    -       99     -


 178       0.01      2,3,5-TRIMETHYLNAPHTHALENE  2245387
 155     1.38  4.59   1.78  0.69    0.72           0.13           2.05
 170     1.90  6.31   2.44  0.95    0.99           0.18           2.81

 179       0.01      ANTHRACENE       120127
 178     2.24  7.59   3.08  1.19    1.13           0.25           3.35

 180       0.01      PYRENE       129000
 202     3.59 11.47   4.95  1.90    1.80           0.40           5.36

 181       0.01      9,10-DIMETHYLANTHRACENE     781431
 191     0.96  3.19   1.24  0.48    0.50           0.09           1.42
 206     2.06  6.86   2.67  1.03    1.08           0.19           3.06

 182       0.01      CHRYSENE  218019
 228     1.61  5.34   2.07  0.80    0.81           0.15           2.39

 183       0.01      PERYLENE        198550
 252     1.11  3.72   1.53  0.59    0.47           0.12           1.65

 184       0.01      DICYANOBUTANE    111693
  41     0.48  1.59   0.62  0.24    0.25           0.05           0.71
  54     0.22  0.71   0.28  0.11    0.11           0.02           0.32

 185       0.01      BUTYLCARBAMATE  14994775
  41     0.35  1.16   0.50  0.09    0.15           0.04           0.52
  59     0.19  0.63   0.27  0.11    0.08           0.02           0.28

 186       0.01      DIBUTYLDISULFIDE 110065
  41     0.54  1.78   0.78  0.31    0.20           0.06           0.82
  57     2.21  7.62   3.29  1.27    1.00           0.24           3.42

 187       0.01      BIS(2-CHLOROETHYL)ETHANE 112265
  63     1.27  4.23   1.83  0.71    0.56           0.13           1.91
  93     0.61  2.08   0.90  0.35    0.27           0.06           0.94

 188       0.01      TRIBUTYLPHOSPHATE 126738
  99     2.81  9.43   3.87  1.49    1.41           0.31           4.19
 155     0.61  2.05   0.84  0.32    0.31           0.07           0.91

 189       0.01      ALDRIN      309002
  66     0.99  3.28   1.27  0.49    0.51           0.09           1.46
 263     0.44  1.47   0.57  0.22    0.23           0.04           0.66

 190       0.01      DIHYDROBENZOFURAN    496162
  91     0.27  1.59   0.65  0.25    0.24           0.05           0.71
 120     0.68  2.27   0.90  0.35    0.33           0.07           0.98

 191       0.01      NITROBENZENE    98953
  77     0.61  2.07   0.80  0.31    0.33           0.06           0.94
 123     0.38  1.30   0.50  0.20    0.21           0.04           0.59
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               Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56        Std #57        Std #58
Mass     109   236    136    -       82   128       98   116       84   112


 192      0.01      BENZOTHIAZOLE    95169
 135   1.56  1.21    0.29          1.71  2.76    1.11  1.86    3.47  2.55

 193      0.01      PHENYLCARBAMATE    102090
  94   1.25  0.96    0.23          1.44  2.23    0.79  1.31    2.88  2.06
 137   0.02  0.01    0.00          0.02  0.03    0.01  0.02    0.04  0.03

 194      0.01      2,4-DINITROTOLUENE   121142
  89   0.35  0.28    0.06          0.40  0.65    0.26  0.44    0.81  0.60
 165   0.71  0.53    0.13          0.75  1.21    0.46  0.76    1.53  1.13

 195      0.01      BENZYLSULFIDE  538749
  91   3.55  2.68    0.63          4.00  6.38    2.10  3.49    9.99  7.42
 123   0.90  0.68    0.16          1.02  1.62    0.53  0.89    2.54  1.88

 196      0.01      DIPHENYLSULFONE  127639
 125   3.82  3.44    0.81          5.16  8.21    2.71  4.51   12.95  8.65
 218   0.92  0.73    0.17          1.10  1.75    0.58  0.96    2.74  2.03

 197      0.01      TRIPHENYLPHOSPHATE  115866
 325   2.59  2.01    0.13          0.79  1.28    0.52  0.87    1.61  1.18
 326   0.09  0.07    0.17          1.03  1.67    0.68  1.14    2.09  1.54

 198      0.01      DIPHENYLMERCURY  587859
  77   0.72  0.56    0.48          2.85  4.59    1.96  3.28    6.08  4.47
 356   0.95  0.74    0.02          0.09  0.15    0.06  0.11    0.20  0.15

 199      0.01      TETRAPHENYLTIN
 197   1.40  1.13    0.27          1.70  2.71    0.89  1.47    4.21  3.13
 351   1.30  1.05    0.25          1.58  2.51    0.82  1.37    3.91  2.91

 200      0.01      BENZYLCHLORIDE         100447
  91   1.55  1.18    0.28          1.77  2.82    0.93  1.54    4.42  3.28
 126   0.42  0.32    0.08          0.48  0.76    0.25  0.42    1.20  0.89

 201      0.01      4-CHLOROBENZONITRILE   623030
 102   0.55  0.42    0.10          0.63  0.99    0.33  0.55    1.57  1.16
 137   2.10  1.57    0.36          2.38  3.79    1.25  2.08    5.95  4.40

 202      0.01      3-CHLOROBENZALDEHYDE   587042
 111   0.06  0.05    0.01          0.08  0.12    0.04  0.07    0.20  0.14
 139   0.12  0.10    0.02          0.15  0.24    0.08  0.13    0.38  0.28

 203      0.01      O-CHLOROANISOLE    766518
 127   0.60  0.46    0.11          0.69  1.09    0.36  0.60    1.71  1.27
 142   1.32  1.00    0.24          0.50  2.40    0.79  1.31    3.76  2.78

 204      0.01      CHLOROBENZAMIDE   619567
 139   0.70  0.55    0.13          0.77  1.25    0.50  0.84    1.57  1.16
 155   0.38  0.30    0.07          0.42  0.68    0.27  0.46    0.85  0.63
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           Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery    Compound Name
          Std #59       Std #60       Std #61       Std #62       Std #63
Mass     110   125     82   110     264    -      188    -       99    -


 192       0.01      BENZOTHIAZOLE    95169
 135    1.14  3.76    1.46  0.57    0.59          0.11          1.68

 193       0.01      PHENYLCARBAMATE    102090
  94    0.87  2.92    1.20  0.46    0.44          0.10          1.30
 137    0.01  0.04    0.01  0.01    0.00          0.00          0.02

 194       0.01      2,4-DINITROTOLUENE   121142
  89    0.27  0.88    0.34  0.13    0.14          0.03          0.39
 165    0.50  1.66    0.64  0.25    0.26          0.05          0.74

 195       0.01      BENZYLSULFIDE  538749
  91    2.47  8.62    3.72  1.44    1.11          0.27          3.90
 123    0.63  2.19    0.94  0.37    0.28          0.07          0.99

 196       0.01      DIPHENYLSULFONE  127639
 125    3.00 11.09    4.77  1.85    1.22          0.35          5.05
 218    0.67  2.36    1.02  0.29    0.30          0.07          1.07

 197       0.01      TRIPHENYLPHOSPHATE  115866
 325    1.98  6.58    2.55  0.95    1.03          0.18          0.78
 326    0.06  0.22    0.08  0.03    0.03          0.01          1.02

 198       0.01      DIPHENYLMERCURY  587859
  77    0.53  1.75    0.68  0.26    0.26          0.05          2.94
 356    0.69  2.28    0.88  0.34    0.35          0.06          0.10

 199       0.01      TETRAPHENYLTIN
 197    1.10  3.66    1.57  0.61    0.44          0.11          1.56
 351    1.03  3.40    1.46  0.57    0.41          0.11          1.54

 200       0.01      BENZYLCHLORIDE          100447
  91    1.10  3.81    1.64  0.64    0.50          0.12          1.71
 126    0.30  1.03    0.45  0.17    0.12          0.03          0.47

 201       0.01      4-CHLOROBENZONITRILE   623030
 102    0.39  1.35    0.58  0.23    0.18          0.04          0.61
 137    1.49  5.12    2.21  0.85    0.67          0.16          2.32

 202       0.01      3-CHLOROBENZALDEHYDE   587042
 111    0.05  0.17    0.07  0.03    0.02          0.00          0.08
 139    0.10  0.32    0.14  0.05    0.04          0.01          0.15

 203       0.01      O-CHLOROANISOLE    766518
 127    0.43  1.48    0.64  0.25    0.17          0.05          0.67
 142    0.94  3.24    1.40  0.54    0.36          0.10          1.46

 204       0.01      CHLOROBENZAMIDE   619567
 139    0.51  1.70    0.66  0.26    0.27          0.05          0.76
 155    0.28  0.92    0.36  0.14    0.15          0.03          0.41
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                 Internal/External Standard File for Cmpd Class # 7

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54        Std #56        Std #57        Std #58
Mass     109   236    136    -       82   128       98   116       84   112


 205       0.01     3,4-DICHLOROBENZALDEHYDE      6287383
 173    0.48  0.39   0.09           0.58  0.93    0.31  0.57    1.46  1.07
 174    0.32  0.26   0.06           0.39  0.62    0.21  0.34    0.98  0.72

 206       0.01     1,2,4-TRICHLOROBENZENE       120821
 145    0.34  0.26   0.06           0.40  0.63    0.22  0.36    0.80  0.57
 180    1.30  1.00   0.24           1.50  2.40    0.83  1.37    3.03  2.16

 207       0.01     2-BROMO-1-CHLOROBENZENE      694804
 190    0.78  0.61   0.14           0.85  1.38    0.55  0.92    1.74  1.28
 192    1.04  0.81   0.19           1.14  1.84    0.74  1.24    2.33  1.71

 208       0.01     1,2-DICHLORONAPHTHALENE   2050693
 161    0.44  0.34   0.08           0.50  0.78    0.28  0.46    1.01  0.72
 196    2.17  1.67   0.40           2.51  3.88    1.38  2.29    5.03  3.58

 209       0.01     1,2,4,5-TETRACHLOROBENZENE  95943
 214    1.18  0.90   0.22           1.29  2.09    0.84  1.40    2.63  1.94
 216    1.54  1.18   0.28           1.69  2.72    1.09  1.83    3.43  2.52

 210       0.01     P-DIBROMOBENZENE   106376
 234    0.68  0.52   0.12           0.77  1.23    0.41  0.67    1.93  1.43
 236    1.29  1.00   0.23           1.48  2.36    0.78  1.30    3.77  2.93

 211       0.01     4-BROMODIPHENYLETHER   6452499
 248    1.08  0.81   0.20           1.19  1.92    0.77  1.29    2.42  1.78
 250    1.13  0.88   0.21           1.26  2.04    0.82  1.37    2.57  1.89

 212       0.01     HEXACHLOROBENZENE  118741
 284    0.74  0.56   0.13           0.84  1.34    0.44  0.73    2.10  1.55
 286    0.60  0.46   0.11           0.68  1.08    0.36  0.59    1.70  1.26

 213       0.01     METHYLSTEARATE          112618
  74    3.42  2.65   0.63           3.89  6.28    2.54  4.25    7.90  5.81
  87    2.22  1.72   0.41           2.52  4.07    1.65  2.76    5.13  3.77
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          Internal/External Standard File for Cmpd Class # 7

Cmpd#   Recovery   Compound Name
         Std #59      Std #60      Std #61       Std #62      Std #63
Mass    110   125     82   110     264    -      188   -      99    -


  205     0.01     3,4-DICHLOROBENZALDEHYDE     6287383
 173   0.37  1.25   0.54  0.21   0.17          0.04         0.57
 174   0.25  0.84   0.36  0.14   0.11          0.03         0.38

  206     0.01     1,2,4-TRICHLOROBENZENE      120821
 145   0.24  0.80   0.33  0.13   0.12          0.03         0.36
 180   0.89  3.05   1.25  0.48   0.46          0.10         1.36

  207     0.01     2-BROMO-1-CHLOROBENZENE     694804
 190   0.57  1.88   0.73  0.28   0.30          0.05         0.84
 192   0.76  2.52   0.98  0.38   0.40          0.07         1.12

  208     0.01     1,2-DICHLORONAPHTHALENE   2050693
 161   0.31  1.02   0.42  0.16   0.15          0.03         0.46
 196   1.52  5.08   2.08  0.80   0.76          0.17         2.27

  209     0.01     1,2,4,5-TETRACHLOROBENZENE   95943
 214   0.86  2.85   1.11  0.43   0.45          0.08         1.27
 216   1.12  3.72   1.44  0.56   0.58          0.11         1.66

  210     0.01     P-DIBROMOBENZENE    106376
 234   0.49  1.66   0.72  0.28   0.19          0.05         0.75
 236   0.93  3.18   1.38  0.53   0.45          0.10         1.45

  211     0.01     4-BROMODIPHENYLETHER    6452499
 248   0.79  2.61   1.01  0.39   0.41          0.07         1.17
 250   0.84  2.78   1.08  0.42   0.44          0.08         1.24

  212     0.01     HEXACHLOROBENZENE   118741
 284   0.53  1.83   0.78  0.30   0.24          0.06         0.82
 286   0.43  1.46   0.63  0.24   0.19          0.05         0.66

  213     0.01     METHYLSTEARATE       112618
  74   2.58  8.56   3.32  1.29   1.33          0.24         3.83
  87   1.67  5.55   2.15  0.83   0.87          0.16         2.48
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Table B-8. RMRs AND RECOVERIES FOR WABN COMPOUNDS (ACCUMULATOR COLUMN, pH 8.0)

Class No. 8

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
54	d_8-Naphthalene (internal)
56	d_5-Nitrobenzene (internal)
57	d_{10}-o-Xylene (internal)
58	d_5-Phenylethanol (internal)
59	d_5-Acetophenone (internal)
60	d_5-Propiophenone (internal)
61	d_{12}-Perylene (internal)
62	d_9-Acridine (internal)
63	d_5-Phenol (internal)

MATRIX OF STANDARD ION RMRs

			Standard							
			d_5-Phenol	d_{10}-o-Xylene		d_8-Naphthalene	d_5-Nitrobenzene		d_5-Phenylethanol	
Compound	Ion	Recovery	m/z 99	m/z 98	m/z 116	m/z 136	m/z 82	m/z 128	m/z 84	m/z 112
d_5-phenol	99	0.55	-	.59(9)	.99(9)	.17(6)	1.04(5)	1.66(3)	2.44(15)	1.75(15)
d_{10}-o-xylene	98 116	0.76 0.76	1.72(9)[a] 1.03(a)	- .60(0)	1.67(1) -	.29(6) .18(6)	1.79(8) 1.07(8)	2.84(8) 1.71(8)	4.21(22) 2.53(22)	3.02(21) 1.81(21)
d_8-naphthalene	136	0.79	5.97(4)	3.51(7)	5.85(7)	-	6.21(3)	9.98(3)	14.63(15)	10.59(18)
d_5-nitrobenzene	82 128	0.82 0.82	.97(4) .61(2)	.57(10) .35(9)	.95(10) .59(9)	.16(3) .10(1)	- .63(1)	1.60(1) -	2.35(17) 1.47(16)	1.70(16) 1.07(15)
d_5-phenylethanol	84 112	0.78 0.78	.42(15) .58(15)	.25(24) .35(22)	.42(24) .58(23)	.071 ~~.54~~(18) .098(18)	.44(16) .61(16)	.70(15) .95(16)	- 1.39(2)	.73(2) -
d_5-propiophenone	82 110	0.93 0.93	1.09(4) 2.85(5)	.65(13) 1.67(13)	1.07(14) 2.78(14)	.18(8) .48(17)	1.13(6) 2.94(6)	1.82(6) 4.72(6)	2.63(11) 6.84(12)	1.90(10) 4.95(11)
d_5-acetophenone	110 125	0.87 0.87	1.52(2) .46(2)	.90(7) .27(8)	1.50(8) .45(7)	.25(4) .76(3) .076	1.60(5) .48(3)	2.55(1) .76(4)	3.71(17) 1.11(18)	2.68(16) .81(17)
d_{12}-perylene	264	0.62	3.56(13)	2.09(7)	3.48(8)	.60(9)	3.70(11)	5.90(12)	8.52(25)	6.37(28)
d_9-acridine	188	0.87	1.45(7)	.86(15)	1.43(15)	.24(8)	1.51(6)	2.40(6)	3.52(13)	2.55(13)
4-fluoro-2-iodotoluene	109 236	NA NA	1.10(4) 1.43(4)	.65(7) .64(6)	1.08(8) 1.39(7)	.18(3) .24(6)	1.14(2) 1.48(3)	1.82(2) 2.37(3)	2.69(18) 3.48(18)	1.97(19) 2.52(18)

(continued)

Compound	Ion	Recovery	Standard							
			d_5-Propiophenone		d_5 Acetophenone		d_{12}-Perylene	d_9-Acridine	4-Fluoro-2-Iodotoluene	
			m/z 82	m/z 110	m/z 110	m/z 125	m/z 264	m/z 188	m/z 109	m/z 236
d_5-phenol	99	0.55	.92(5)	.35(5)	.67(2)	2.21(3)	.31(15)	.70(7)	.91(5)	.71(4)
d_{10}-o-xylene	98	0.76	1.59(12)	.61(13)	1.13(7)	3.77(7)	.53(10)	1.20(13)	1.56(6)	1.21(6)
	116	0.76	.95(13)	.37(12)	.67(6)	2.27(7)	.32(10)	.72(13)	.94(6)	.73(6)
d_8-naphthalene	136	0.79	5.51(8)	2.13(8)	3.91(4)	13.14(3)	1.76(15)	4.20(8)	5.45(1)	4.20(1)
d_5-nitrobenzene	82	0.82	.89(6)	.34(6)	.63(4)	2.12(4)	.29(19)	.67(6)	.88(2)	.68(3)
	128	0.82	.55(6)	.22(6)	.39(1)	1.32(3)	.18(20)	.42(6)	.55(3)	.42(3)
d_5-phenylethanol	84	0.78	.39(11)	.15(10)	.28(16)	.93(12)	.13(28)	.29(11)	.38(18)	.30(17)
	112	0.78	.53(10)	.21(9)	.39(16)	1.28(16)	.18(28)	.41(13)	.52(19)	.42(16)
d_5-propiophenone	82	0.93	-	.39(1)	.71(7)	2.40(6)	.33(23)	.76(5)	1.00(7)	.77(7)
	110	0.93	2.60(1)	-	1.85(6)	6.21(6)	.87(19)	2.00(5)	2.59(7)	1.99(7)
d_5-acetophenone	110	0.87	1.41(6)	.55(6)	-	3.39(1)	.47(14)	1.10(9)	1.37(4)	1.07(2)
	125	0.87	.42(6)	.16(5)	.30(2)	-	.14(18)	.32(9)	.42(2)	.32(3)
d_{12}-perylene	264	0.62	3.08(14)	1.27(16)	2.37(12)	7.91(12)	-	2.50(16)	3.21(9)	2.51(9)
d_9-acridine	188	0.87	1.33(5)	.52(5)	.95(10)	3.15(11)	.39(40)	-	1.32(8)	1.03(8)
4-fluoro-2-iodotoluene	109	NA	1.01(7)	.39(7)	.71(2)	2.40(2)	.34(12)	.76(8)	-	.77(1)
	236	NA	1.31(7)	.51(7)	.92(3)	3.11(2)	.42(16)	1.00(8)	1.30(1)	-

[a] (CV).

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                        Internal/External Standard File for Cmpd Class # 8

Cmpd#   Recovery   Compound Name
         Std # 2      Std #54      Std #56      Std #57       Std #61
Mass    109    236    136    -      82    128     98    116    264    -


  100     0.01      PYRIDINE       110861
  52   0.29  0.22    0.05         0.33  0.51   0.19  0.32
  79   0.44  0.34    0.08         0.51  0.78   0.30  0.50

  101     0.36      ALPHA-PICOLINE    109068
  66   0.26  0.20    0.05         0.30  0.46   0.16  0.27
  93   0.66  0.51    0.12         0.76  1.18   0.40  0.66

  102     0.34      ANILINE     62533
  66   0.23  0.19    0.04         0.28  0.41   0.15  0.24
  93   0.76  0.54    0.13         0.81  1.25   0.45  0.74

  103     0.95      LUTIDINE    108485
 106   0.13  0.10    0.02         0.15  0.25   0.08  0.13
 107   0.22  0.16    0.04         0.24  0.39   0.13  0.21

  104     0.01      TOLUIDINE  106490
 106   0.89  0.69    0.16         0.97  1.57   0.64  1.07
 107   0.71  0.56    0.13         0.78  1.27   0.51  0.86

  105     0.95      INDOLE  120729
  90   0.72  0.54    0.13         0.82  1.30   0.43  0.71
 117   1.92  1.45    0.34                      1.14  1.89   0.61

  106     0.84      2,3,6-TRIMETHYLPYRIDINE   1462846
 120   0.66  0.51    0.12         0.76  1.18   0.42  0.69
 121   0.90  0.69    0.17         1.03  1.61   0.55  0.91

  107     0.87      2,6-DIMETHYLANILINE 1300738
 106   0.36  0.27    0.06         0.41  0.65   0.21  0.36
 121   0.57  0.44    0.10         0.66  1.04   0.34  0.57

  108     0.95      M-CHLOROANILINE     108429
 127   1.09  0.84    0.20         1.26  1.94   0.69  1.15
 129   0.34  0.26    0.06         0.29  0.60   0.22  0.36

  109     0.91      QUINOLINE      91225
 129   1.82  1.41    0.34         1.99  3.22   1.30  2.17

  110     0.77      P-NITROANILINE     100016
  65   0.44  0.35    0.08         0.52  0.83   0.27  0.46
 138   0.56  0.45    0.11         0.67  1.07   0.35  0.58

  111     0.90      2,4-DIMETHYLQUINOLINE   1198374
 156   0.41  0.32    0.08         0.47  0.75   0.26  0.43
 157   2.01  1.54    0.37         2.31  3.59   1.27  2.11

  112     0.01      1,8-DIAMINONAPHTHALENE
 114   0.03  0.02    0.00         0.04  0.06   0.02  0.03
 141   0.05  0.04    0.01         0.06  0.01   0.03  0.05
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            Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery    Compound Name
          Std #62       Std #63
Mass      188    -       99    -


  100      0.01      PYRIDINE       110861
  52     0.02         0.30
  79     0.04         0.50

  101      0.36      ALPHA-PICOLINE    109068
  66     0.02         0.27
  93     0.05         0.69

  102      0.34      ANILINE     62533
  66     0.02         0.24
  93     0.05         0.73

  103      0.95      LUTIDINE    108485
 106     0.01         0.15
 107     0.02         0.24

  104      0.01      TOLUIDINE  106490
 106     0.06         0.96
 107     0.05         0.77

  105      0.95      INDOLE  120729
  90     0.05         0.79
 117     0.15         2.12

  106      0.84      2,3,6-TRIMETHYLPYRIDINE   1462846
 120     0.05         0.67
 121     0.07         0.94

  107      0.87      2,6-DIMETHYLANILINE 1300738
 106     0.03         0.40
 121     0.04         0.64

  108      0.95      M-CHLOROANILINE     108429
 127     0.98         1.14
 129     0.03         0.35

  109      0.91      QUINOLINE      91225
 129     0.12         1.96

  110      0.77      P-NITROANILINE     100016
  65     0.04         0.51
 138     0.05         0.65

  111      0.90      2,4-DIMETHYLQUINOLINE   1198374
 156     0.03         0.43
 157     0.15         2.09

  112      0.01      1,8-DIAMINONAPHTHALENE
 114     0.00         0.03
 141     0.00         0.55
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           Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54       Std #56       Std #57       Std #61
Mass     109   236     136    -      82   128      98   116     264    -


 113       0.62      NICOTINE    54115
  84    1.17  0.90    0.22          1.35  2.09    0.74  1.23
 133    0.28  0.21    0.05          0.32  0.49    0.17  0.29

 114       0.82      CARBAZOLE   86748
 167    3.73  2.88    0.69          4.30  6.66    2.37  3.92

 115       0.82      2-AMINOBIPHENYL       90415
 168    6.79  5.11    1.20          7.65 12.18    4.61  6.67
 169   12.72  9.45    2.22         14.15 22.54    7.42 12.30

 116       0.85      DIPHENYLAMINE     122394
 168    1.48  1.14    0.27          1.71  2.65    0.94  1.56
 169    2.79  2.15    0.52          3.22  4.99    1.77  2.93

 117       0.01      DICYCLOHEXYLAMINE    101837
  56    0.33  0.37    0.06          0.39  0.63    0.21  0.35
 138    0.96  0.76    0.18          1.12  1.80    0.61  1.02

 118       0.82      TRIBUTYLAMINE     102829
 100    0.42  0.33    0.08          0.49  0.75    0.27  0.44
 142    1.53  1.18    0.28          1.77  2.74    0.97  1.61

 119       0.86      CAFFEINE       58082
 109    0.10  0.08    0.02          0.12  0.17    0.06  0.10
 194    0.19  0.15    0.04          0.22  0.34    0.12  0.20

 120       0.50      DIBENZYLAMINE  103491
  91    1.62  1.26    0.30          1.78  2.87    1.16  1.94
 197    0.13  0.11    0.03          0.15  0.24    0.10  0.16

 121       0.69      N,N-DIMETHYLDODECYLAMINE    112185
  58    4.72  3.88    0.87          5.47  8.83    3.58  5.99
  59    0.17  0.13    0.03          0.20  0.30    0.13  0.21

 122       0.71      ATRAZINE 1912249
 200    2.75  2.20    0.52          3.28  5.23    1.72  2.86
 215    1.67  1.34    0.31          2.00  3.18    1.05  1.74

 123       0.66      HEPTANONE(2)      110430
  43    1.21  0.94    0.22          1.33  2.14    0.85  1.14
  58    0.75  0.58    0.14          0.83  1.33    0.53  0.88

 124       0.01      BUTOXYETHANOL     111762
  41    0.21  0.17    0.04          0.25  0.40    0.13  0.22
  57    0.55  0.42    0.10          0.63  1.03    0.35  0.58

 125       0.77      2-OCTANONE    111137
  43    1.30  1.01    0.24          1.43  2.31    0.91  1.53
  58    1.02  0.79    0.19          1.11  1.80    0.71  1.19
```

```
        Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery   Compound Name
          Std #62     Std #63
Mass      188    -    99    -


 113       0.62      NICOTINE    54115
  84     0.09         1.22
 133     0.02         0.29

 114       0.82      CARBAZOLE   86748
 167     0.31         4.22

 115       0.82      2-AMINOBIPHENYL     90415
 168     0.51         7.45
 169     0.95        13.80

 116       0.85      DIPHENYLAMINE    122394
 168     0.11         1.55
 169     0.22         2.91

 117       0.01      DICYCLOHEXYLAMINE   101837
  56     0.03         0.38
 138     0.08         1.09

 118       0.82      TRIBUTYLAMINE    102829
 100     0.03         0.44
 142     0.12         1.59

 119       0.86      CAFFEINE      58082
 109     0.01         0.10
 194     0.02         0.21

 120       0.50      DIBENZYLAMINE  103491
  91     0.11         1.74
 197     0.01         0.14

 121       0.69      N,N-DIMETHYLDODECYLAMINE   112185
  58     0.34         5.37
  59     0.01         0.19

 122       0.71      ATRAZINE 1912249
 200     0.22         3.26
 215     0.13         1.95

 123       0.66      HEPTANONE(2)     110430
  43     0.08         1.30
  58     0.05         0.81

 124       0.01      BUTOXYETHANOL    111762
  41     0.02         0.22
  57     0.04         0.57

 125       0.77      2-OCTANONE   111137
  43     0.09         1.40
  58     0.07         1.09
```

```
          Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery    Compound Name
          Std # 2      Std #54      Std #56      Std #57      Std #61
Mass      109   236    136    -     82   128     98   116    264    -


  126      0.52      BUTYLPROPIONATE      590012
  57     1.48  1.14   0.27           1.71  2.73   0.90  1.49
  75     0.44  0.34   0.08           0.51  0.82   0.27  0.45

  127      0.85      ISOPHORONE     78591
  82     1.77  1.36   0.33           2.04  3.17   1.13  1.86
 138     0.39  0.30   0.07           0.45  0.72   0.25  0.41

  128      0.64      FENCHONE       1195759
  69     0.66  0.51   0.12           0.72  1.17   0.47  0.78
  81     1.44  1.12   0.27           1.58  2.55   1.02  1.71

  129      0.92      ALPHA-TERPINEOL    98555
  59     0.56  0.43   0.10           0.65  1.00   0.36  0.59
 136     0.32  0.25   0.06           0.37  0.58   0.21  0.34

  130      0.94      N-DECANOL  112301
  41     0.40  0.31   0.07           0.46  0.74   0.25  0.42
  43     0.44  0.34   0.08           0.51  0.79   0.28  0.46

  131      0.91      DIMETHYLADIPATE      627930
  59     0.56  0.45   0.10           0.64  1.03   0.41  0.69
 114     0.44  0.35   0.08           0.49  0.79   0.32  0.54

  132      0.45      METHYLSTEARATE       112618
  74     3.42  2.65   0.63           3.89  6.28   2.54  4.25
  87     2.22  1.72   0.41           2.52  4.07   1.65  2.76

  133      0.01      N-DECANE  124185
  43     1.47  1.11   0.26           1.67  2.66   0.88  1.46
  57     1.42  1.08   0.25           1.64  2.61   0.85  1.41

  134      0.44      N-TRIDECANE 629505
  43     2.18  1.64   0.34           2.48  3.95   1.30  2.16
  57     2.75  2.09   0.50           3.14  5.01   1.66  2.77

  135      0.42      N-TETRADECANE    629594
  43     2.52  1.92   0.45           2.88  4.58   1.51  2.51
  57     3.40  2.55   0.61           3.87  6.16   2.03  3.37

  136      0.01      N-PENTADECANE    692692
  57     2.78  2.14   0.52           3.22  4.99   1.77  2.94
  71     1.73  1.33   0.32           2.01  3.11   1.10  1.83

  137      0.45      N-HEXADECANE     544763
  43     1.90  1.45   0.34           2.16  3.45   1.13  1.89
  57     2.72  2.08   0.49           3.11  4.96   1.63  2.71

  138      0.01      N-HEPTADECANE 629787
  57     3.13  2.41   0.58           3.61  5.59   1.99  3.30
  71     2.07  1.60   0.38           2.39  3.70   1.32  2.18
```

```
          Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery    Compound Name
          Std #62       Std #63
Mass     188    -       99    -


  126      0.52      BUTYLPROPIONATE      590012
  57    0.12          1.66
  75    0.04          0.50

  127      0.85      ISOPHORONE    78591
  82    0.14          1.80
 138    0.03          0.41

  128      0.64      FENCHONE      1195759
  69    0.05          0.71
  81    0.10          1.55

  129      0.92      ALPHA-TERPINEOL   98555
  59    0.04          0.58
 136    0.03          0.34

  130      0.94      N-DECANOL  112301
  41    0.03          0.41
  43    0.03          0.46

  131      0.91      DIMETHYLADIPATE      627930
  59    0.04          0.62
 114    0.03          0.48

  132      0.45      METHYLSTEARATE       112618
  74    0.24          3.83
  87    0.16          2.48

  133      0.01      N-DECANE  124185
  43    0.11          1.62
  57    0.11          1.58

  134      0.44      N-TRIDECANE 629505
  43    0.17          2.41
  57    0.21          3.09

  135      0.42      N-TETRADECANE   629594
  43    0.19          2.80
  57    0.26          3.77

  136      0.01      N-PENTADECANE   692692
  57    0.22          2.92
  71    0.14          1.82

  137      0.45      N-HEXADECANE    544763
  43    0.15          2.11
  57    0.21          3.03

  138      0.01      N-HEPTADECANE 629787
  57    0.24          3.27
  71    0.16          2.17
```

```
              Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery     Compound Name
          Std # 2      Std #54         Std #56         Std #57        Std #61
Mass     109    236    136    -        82    128       98    116      264    -


  139       0.01      N-OCTADECANE     593453
   57    2.99  2.51    0.59           3.75  5.98     1.88  3.14
   71    1.98  1.66    0.39           2.48  3.95     1.25  2.08

  140       0.47      N-NONADECANE   629925
   71    2.12  1.61    0.38           2.42  3.85     1.27  2.11
   85    1.42  1.08    0.25           1.61  2.57     0.85  1.41

  141       0.08      N-EICOSANE  1112958
   57    4.43  3.41    0.82           5.11  7.92     2.82  4.66
   71    3.03  2.33    0.56           3.50  5.43     1.93  3.19

  142       0.63      N-HENEICOSANE         629947
   57    3.93  2.96    0.70           4.43  7.05     2.32  3.86
   71    2.71  2.05    0.48           3.07  4.88     1.61  2.67

  143       0.66      N-DOCOSANE      629970
   57    3.73  2.98    0.70           4.46  7.10     2.33  3.88
   71    2.60  2.08    0.49           3.11  4.96     1.63  2.70

  144       0.66      N-TRICOSANE      638675
   57    3.99  3.19    0.75           4.77  7.60     2.49  4.14
   71    2.80  2.24    0.53           3.35  5.34     1.75  2.91

  145       0.74      PHENYLACETATE     122792
   94    1.84  1.43    0.34           2.01  3.25     1.30  2.18
  136    0.25  0.20    0.05           0.28  0.45     0.18  0.30

  146       0.79      BENZYLACETATE        140114
   91    0.52  0.40    0.09           0.57  0.92     0.37  0.62
  108    1.09  0.85    0.20           1.19  1.92     0.77  1.29

  147       0.36      METHYLBENZENESULFONATE
   77    1.24  0.94    0.22           1.41  2.25     0.74  1.23
  172    0.44  0.34    0.08           0.50  0.80     0.26  0.44

  148       0.46      METHYLTOLUENESULFONATE
   91    1.60  1.21    0.29           1.81  2.89     0.95  1.58
  155    0.72  0.54    0.13           0.81  1.29     0.42  0.71

  149       0.74      DIMETHYLPHTHALATE          131113
   77    0.81  0.63    0.15           0.94  1.45     0.52  0.85
  163    5.29  4.07    0.98           6.10  9.46     3.36  5.56

  150       0.53      ETHYLTOLUENESULFONATE
   91    1.74  1.32    0.31           1.97  3.14     1.03  1.72
  155    1.18  0.94    0.22           1.40  2.23     0.73  1.21

  151       0.87      DIETHYLPHTHALATE      84662
  149    3.19  2.43    0.57           3.65  5.79     1.90  3.17
  177    0.80  0.61    0.14           0.93  1.47     0.48  0.80
```

```
              Internal/External Standard File for Cmpd Class # 8

    Cmpd#    Recovery    Compound Name
              Std #62      Std #63
    Mass     188    -      99    -


      139       0.01     N-OCTADECANE     593453
      57     0.24         3.65
      71     0.06         2.41

      140       0.47     N-NONADECANE   629925
      71     0.16         2.35
      85     0.11         1.57

      141       0.08     N-EICOSANE  1112958
      57     0.35         4.63
      71     0.23         3.17

      142       0.63     N-HENEICOSANE         629947
      57     0.30         4.31
      71     0.21         2.99

      143       0.66     N-DOCOSANE      629970
      57     0.30         4.35
      71     0.21         3.04

      144       0.66     N-TRICOSANE      638675
      57     0.32         4.65
      71     0.22         3.27

      145       0.74     PHENYLACETATE     122792
      94     0.13         1.98
     136     0.02         0.28

      146       0.79     BENZYLACETATE       140114
      91     0.04         0.56
     108     0.07         1.17

      147       0.36     METHYLBENZENESULFONATE
      77     0.09         1.38
     172     0.03         0.49

      148       0.46     METHYLTOLUENESULFONATE
      91     0.12         1.76
     155     0.05         0.79

      149       0.74     DIMETHYLPHTHALATE        131113
      77     0.06         0.85
     163     0.41         5.51

      150       0.53     ETHYLTOLUENESULFONATE
      91     0.13         1.92
     155     0.09         1.36

      151       0.87     DIETHYLPHTHALATE    84662
     149     0.24         3.54
     177     0.06         0.89
```

```
                 Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery   Compound Name
           Std # 2     Std #54        Std #56        Std #57        Std #61
Mass      109   236    136    -        82   128       98   116      264    -


  152        0.01     DIBUTYLPHTHALATE     84742
   57     0.29  0.23   0.05           0.34  0.52    0.19  0.31
  149     7.17  5.52   1.33           8.27 12.80    4.55  7.54

  153        0.64     BUTYLBENZYLPHTHALATE
   91     2.09  1.62   0.38           2.28  3.69    1.48  2.48
  149     3.37  2.62   0.62           3.69  5.95    2.40  4.01

  154        0.74     DIETHYLHEXYLPHTHALATE      117817
  149     5.22  4.07   0.96           5.71  9.23    3.74  6.26
  167     1.98  1.54   0.37           2.17  3.51    1.42  2.37

  155        0.01     BENZALDEHYDE    100527
   77     0.36  0.28   0.07           0.42  0.64    0.23  0.38
  105     0.40  0.31   0.07           0.46  0.70    0.25  0.42

  156        0.88     TOLUALDEHYDE    529204
   91     0.54  0.44   0.10           0.65  1.04    0.34  0.57
  119     0.63  0.51   0.12           0.77  1.23    0.41  0.68

  157        0.92     ACETOPHENONE          98862
   77     0.38  0.64   0.15           0.96  1.53    0.53  0.87
  105     1.22  0.94   0.23           1.41  2.25    0.78  1.29

  158        0.01     SALICYLALDEHYDE         90028
  121     0.56  0.44   0.10           0.61  0.99    0.40  0.67
  122     0.60  0.47   0.11           0.60  1.07    0.43  0.72

  159        0.96     ANISALDEHYDE     123115
  135     1.37  1.08   0.25           1.53  2.47    0.91  1.66
  136     0.60  0.47   0.18           1.07  1.73    0.70  1.16

  160        0.55     PHENOL    108952
   94     1.07  0.84   0.20           1.18  1.90    0.76  1.27

  161        0.63     CRESOL(P)        106445
  107     1.21  0.93   0.23           1.40  2.25    0.80  1.29
  108     1.07  0.82   0.20           1.24  1.99    0.69  1.14

  162        0.95     2,3-DIMETHYLPHENOL  526750
  107     0.87  0.67   0.16           1.00  1.61    0.57  0.95
  122     0.91  0.70   0.17           1.05  1.64    0.58  0.96

  163        0.88     ISOPROPYLPHENOL(O)    88699
  121     1.79  1.36   0.32           2.04  3.25    1.07  1.78
  136     0.07  0.56   0.12           0.75  1.19    0.39  0.65

  164        0.01     O-NITROPHENOL    88755
   65     0.03  0.02   0.00           0.03  0.05    0.02  0.03
  139     0.13  0.10   0.02           0.14  0.23    0.09  0.15
```

```
          Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery    Compound Name
          Std #62       Std #63
Mass      188    -      99    -


  152      0.01      DIBUTYLPHTHALATE     84742
  57    0.02          0.31
 149    0.55          7.47

  153      0.64      BUTYLBENZYLPHTHALATE
  91    0.14          2.24
 149    0.23          3.62

  154      0.74      DIETHYLHEXYLPHTHALATE      117817
 149    0.35          5.61
 167    0.13          2.13

  155      0.01      BENZALDEHYDE    100527
  77    0.03          0.38
 105    0.03          0.42

  156      0.88      TOLUALDEHYDE    529204
  91    0.05          0.64
 119    0.05          0.75

  157      0.92      ACETOPHENONE          98862
  77    0.06          0.87
 105    0.09          1.28

  158      0.01      SALICYLALDEHYDE         90028
 121    0.04          0.60
 122    0.04          0.65

  159      0.96      ANISALDEHYDE     123115
 135    0.09          1.50
 136    0.04          1.05

  160      0.55      PHENOL    108952
  94    0.07          1.15

  161      0.63      CRESOL(P)       106445
 107    0.10          1.31
 108    0.09          1.16

  162      0.95      2,3-DIMETHYLPHENOL  526750
 107    0.07          0.94
 122    0.07          0.95

  163      0.88      ISOPROPYLPHENOL(O)    88699
 121    0.14          1.99
 136    0.05          0.73

  164      0.01      O-NITROPHENOL   88755
  65    0.00          0.03
 139    0.01          0.14
```

```
              Internal/External Standard File for Cmpd Class # 8

Cmpd#     Recovery    Compound Name
           Std # 2      Std #54        Std #56       Std #57       Std #61
Mass      109   236     136    -       82   128      98   116     264    -

 165        0.90      4-CHLORO-3-METHYLPHENOL    59507
 107     0.93  0.71     0.17          1.06  1.68    0.55  0.92
 142     1.02  0.77     0.18          1.16  1.84    0.61  1.01

 166        0.01      4-CHLOROCRESOL
 107     0.83  0.64     0.16          0.97  1.57    0.53  0.88
 142     0.94  0.72     0.17          1.09  1.77    0.60  0.99

 167        0.01      1-NAPHTHOL    90153
 115     0.35  0.26     0.06          0.38  0.61    0.20  0.34
 144     0.61  0.45     0.11          0.67  1.07    0.35  0.29

 168        0.86      P-TERT-BUTYLPHENOL      98544
 107     0.56  0.43     0.10          0.65  1.03    0.34  0.56
 135     1.96  1.49     0.35          2.22  3.54    1.17  1.94

 169        0.32      2-NITROCRESOL     119335
  77     0.26  0.20     0.05          0.30  0.46    0.07  0.27
 153     0.74  0.57     0.14          0.83  1.33    0.46  0.78

 170        0.78      2,4-DICHLOROPHENOL      120832
 162     1.13  0.88     0.21          1.24  2.00    0.80  1.34
 164     0.72  0.53     0.13          0.78  1.27    0.51  0.85

 171        0.66      2,4,6-TRICHLOROPHENOL   88062
 196     0.81  0.63     0.15          0.89  1.44    0.58  0.97
 198     0.83  0.64     0.15          0.91  1.46    0.59  0.98

 172        0.73      DI-TERT-BUTYL-4-METHYLPHENOL  128370
 205     2.53  1.97     0.47          2.78  4.49    1.81  3.03
 220     0.67  0.52     0.12          0.73  1.18    0.48  0.80

 173        0.00      PENTACHLOROPHENOL 87865
 264     0.29  0.22     0.05          0.34  0.54    0.19  0.31
 266     0.47  0.36     0.09          0.55  0.91    0.32  0.54

 174        0.65      2-METHYLNAPHTHALENE    91576
 141     2.03  1.58     0.38          2.23  3.60    1.44  2.42
 142     2.51  1.96     0.46          2.76  4.45    1.79  2.99

 175        0.76      ACENAPHTHENE  83329
 153     1.26  0.98     0.23          1.38  2.22    0.89  1.49
 154     3.40  2.64     0.63          3.73  6.02    2.41  4.04

 176        0.78      BIPHENYL 92524
 154     2.28  1.78     0.42          2.51  4.04    1.63  2.72

 177        0.78      1,8-DIMETHYLNAPHTHALENE  569415
 141     1.59  1.24     0.29          1.74  2.82    1.13  1.89
 156     2.30  1.79     0.42          2.52  4.07    1.63  2.73
```

```
            Internal/External Standard File for Cmpd Class # 8

  Cmpd#    Recovery    Compound Name
            Std #62       Std #63
  Mass     188    -       99    -


   165       0.90     4-CHLORO-3-METHYLPHENOL    59507
  107     0.07         1.03
  142     0.08         1.13

   166       0.01     4-CHLOROCRESOL
  107     0.07         0.91
  142     0.08         1.03

   167       0.01     1-NAPHTHOL   90153
  115     0.03         0.38
  144     0.05         0.66

   168       0.86     P-TERT-BUTYLPHENOL      98544
  107     0.04         0.62
  135     0.15         2.16

   169       0.32     2-NITROCRESOL     119335
   77     0.02         0.27
  153     0.06         0.78

   170       0.78     2,4-DICHLOROPHENOL      120832
  162     0.08         1.22
  164     0.05         0.77

   171       0.66     2,4,6-TRICHLOROPHENOL   88062
  196     0.05         0.88
  198     0.06         0.89

   172       0.73     DI-TERT-BUTYL-4-METHYLPHENOL  128370
  205     0.17         2.73
  220     0.05         0.72

   173       0.00     PENTACHLOROPHENOL 87865
  264     0.02         0.31
  266     0.04         0.50

   174       0.65     2-METHYLNAPHTHALENE   91576
  141     0.14         2.19
  142     0.17         2.71

   175       0.76     ACENAPHTHENE  83329
  153     0.09         1.35
  154     0.23         3.66

   176       0.78     BIPHENYL 92524
  154     0.16         2.46

   177       0.78     1,8-DIMETHYLNAPHTHALENE  569415
  141     0.11         1.71
  156     0.16         2.48
```

```
                  Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery   Compound Name
          Std # 2      Std #54       Std #56         Std #57        Std #61
Mass     109   236    136     -      82    128       98    116     264     -


 178        0.88     FLUORENE      86737
 165    2.74  2.13    0.49           3.01  4.85    1.95  3.27
 166    3.07  2.38    0.57           3.44  5.55    2.23  3.74

 179        0.84     2,3,5-TRIMETHYLNAPHTHALENE  2245387
 155    1.86  1.44    0.34           2.08  3.36    1.36  2.27
 170    2.56  1.99    0.47           2.86  4.62    1.86  3.11

 180        0.78     ANTHRACENE      120127
 178    3.21  2.47    0.60           3.71  5.74    2.04  3.38

 181        0.73     PYRENE     129000
 202    4.88  3.75    0.95           5.66  8.73    3.27  5.18

 182        0.60     9,10-DIMETHYLANTHRACENE  781431
 191    1.33  1.03    0.25           1.45  2.35    0.94  1.57
 206    2.85  2.22    0.53           3.13  5.04    2.01  3.37

 183        0.43     CHRYSENE      218019
 228    2.21  1.73    0.41           2.42  3.92    1.59  2.66

 184        0.62     PERYLENE      198550
 252    1.60  1.23    0.30           1.84  2.86    1.02  1.68

 185        0.71     DICYANOBUTANE  111693
  41    0.66  0.51    0.12           0.72  1.17    0.47  0.79
  54    0.29  0.23    0.05           0.32  0.52    2.10  0.35

 186        0.40     BUTYLCARBAMATE  14994775
  41    0.48  0.36    0.08           0.54  0.86    0.28  0.47
  59    0.24  0.26    0.05           0.29  0.47    0.15  0.25

 187        0.58     DIBUTYLDISULFIDE     110065
  41    0.73  0.56    0.13           0.84  1.34    0.44  0.73
  57    3.09  2.36    0.56           3.54  5.64    1.85  3.09

 188        0.92     BIS(2-CHLOROETHYL)ETHANE     112265
  63    1.71  1.31    0.31           1.97  3.13    1.03  1.71
  93    0.84  0.65    0.15           0.97  1.54    0.51  0.84

 189        0.86     TRIBUTYLPHOSPHATE        126738
  99    4.03  3.10    0.75           4.65  7.20    2.56  4.24
 155    0.88  0.68    0.16           1.01  1.57    0.56  0.92

 190        0.83     ALDRIN     309002
  66    1.33  1.03    0.24           1.49  2.40    0.97  1.62
 263    0.60  0.46    0.11           0.67  1.08    0.44  0.73

 191        0.01     DIHYDROBENZOFURAN  496162
  91    0.68  0.52    0.13           0.79  1.25    0.43  0.72
 120    0.97  0.75    0.18           1.12  1.67    0.66  0.78
```

```
          Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery   Compound Name
          Std #62      Std #63
Mass     188    -      99    -


  178      0.88     FLUORENE     86737
 165   0.19          2.95
 166   0.21          3.38

  179      0.84     2,3,5-TRIMETHYLNAPHTHALENE  2245387
 155   0.13          2.05
 170   0.18          2.81

  180      0.78     ANTHRACENE     120127
 178   0.25          3.35

  181      0.73     PYRENE    129000
 202   0.40          5.36

  182      0.60     9,10-DIMETHYLANTHRACENE  781431
 191   0.09          1.42
 206   0.19          3.06

  183      0.43     CHRYSENE     218019
 228   0.15          2.39

  184      0.62     PERYLENE     198550
 252   0.12          1.65

  185      0.71     DICYANOBUTANE  111693
  41   0.05          0.71
  54   0.02          0.32

  186      0.40     BUTYLCARBAMATE  14994775
  41   0.04          0.52
  59   0.02          0.28

  187      0.58     DIBUTYLDISULFIDE    110065
  41   0.06          0.82
  57   0.24          3.42

  188      0.92     BIS(2-CHLOROETHYL)ETHANE    112265
  63   0.13          1.91
  93   0.06          0.94

  189      0.86     TRIBUTYLPHOSPHATE      126738
  99   0.31          4.19
 155   0.07          0.91

  190      0.83     ALDRIN    309002
  66   0.09          1.46
 263   0.04          0.66

  191      0.01     DIHYDROBENZOFURAN  496162
  91   0.05          0.71
 120   0.07          0.98
```

```
              Internal/External Standard File for Cmpd Class # 8

Cmpd#    Recovery   Compound Name
          Std # 2     Std #54       Std #56      Std #57      Std #61
Mass     109   236    136    -     82   128     98   116     264    -


 192       0.70     NITROBENZENE   98953
  77     0.86  0.67   0.16         0.94  1.51   0.61  1.02
 123     0.54  0.42   0.10         0.59  0.95   0.38  0.64

 193       0.85     BENZOTHIAZOLE    95169
 135     1.56  1.21   0.29         1.71  2.76   1.11  1.86

 194       0.01     PHENYLCARBAMATE 102090
  94     1.25  0.96   0.23         1.44  2.23   0.79  1.31
 137     0.02  0.01   0.00         0.02  0.03   0.01  0.02

 195       0.89     2,4-DINITROTOLUENE 121142
  89     0.35  0.28   0.06         0.40  0.65   0.26  0.44
 165     0.71  0.53   0.13         0.75  1.21   0.46  0.76

 196       0.67     BENZYLSULFIDE     538749
  91     3.55  2.68   0.63         4.00  6.38   2.10  3.49
 123     0.90  0.68   0.16         1.02  1.62   0.53  0.89

 197       0.69     DIPHENYLSULFONE      127639
 125     3.82  3.44   0.81         5.16  8.21   2.71  4.51
 218     0.92  0.73   0.17         1.10  1.75   0.58  0.96

 198       0.81     TRIPHENYLPHOSPHATE    115866
 325     2.59  2.01   0.13         0.79  1.28   0.52  0.87
 326     0.09  0.07   0.17         1.03  1.67   0.68  1.14

 199       0.01     DIPHENYLMERCURY   587859
  77     0.72  0.56   0.48         2.85  4.59   1.96  3.28
 356     0.95  0.74   0.02         0.09  0.15   0.06  0.11

 200       0.47     TETRAPHENYLTIN
 197     1.40  1.13   0.27         1.70  2.71   0.89  1.47
 351     1.30  1.05   0.25         1.58  2.51   0.82  1.37

 201       0.35     BENZYLCHLORIDE       100447
  91     1.55  1.18   0.28         1.77  2.82   0.93  1.54
 126     0.42  0.32   0.08         0.48  0.76   0.25  0.42

 202       0.80     4-CHLOROBENZONITRILE  623030
 102     0.55  0.42   0.10         0.63  0.99   0.33  0.55
 137     2.10  1.57   0.36         2.38  3.79   1.25  2.08

 203       0.01     3-CHLOROBENZALDEHYDE 587042
 111     0.06  0.05   0.01         0.08  0.12   0.04  0.07
 139     0.12  0.10   0.02         0.15  0.24   0.08  0.13

 204       0.57     O-CHLOROANISOLE    766518
 127     0.60  0.46   0.11         0.69  1.09   0.36  0.60
 142     1.32  1.00   0.24         0.50  2.40   0.79  1.31
```

```
           Internal/External Standard File for Cmpd Class # 8

 Cmpd#     Recovery     Compound Name
            Std #62       Std #63
 Mass       188    -      99    -


  192         0.70      NITROBENZENE   98953
   77     0.06           0.94
  123     0.04           0.59

  193         0.85      BENZOTHIAZOLE    95169
  135     0.01           1.68

  194         0.01      PHENYLCARBAMATE 102090
   94     0.10           1.30
  137     0.00           0.02

  195         0.89      2,4-DINITROTOLUENE 121142
   89     0.03           0.39
  165     0.05           0.74

  196         0.67      BENZYLSULFIDE     538749
   91     0.27           3.90
  123     0.07           0.99

  197         0.69      DIPHENYLSULFONE       127639
  125     0.35           5.05
  218     0.07           1.07

  198         0.81      TRIPHENYLPHOSPHATE    115866
  325     0.18           0.78
  326     0.01           1.02

  199         0.01      DIPHENYLMERCURY   587859
   77     0.05           2.94
  356     0.06           0.10

  200         0.47      TETRAPHENYLTIN
  197     0.11           1.56
  351     0.11           1.54

  201         0.35      BENZYLCHLORIDE       100447
   91     0.12           1.71
  126     0.03           0.47

  202         0.80      4-CHLOROBENZONITRILE  623030
  102     0.04           0.61
  137     0.16           2.32

  203         0.01      3-CHLOROBENZALDEHYDE 587042
  111     0.00           0.08
  139     0.01           0.15

  204         0.57      O-CHLOROANISOLE    766518
  127     0.05           0.67
  142     0.10           1.46
```

```
           Internal/External Standard File for Cmpd Class # 8

Cmpd#     Recovery    Compound Name
           Std # 2     Std #54        Std #56        Std #57        Std #61
Mass      109   236    136    -       82   128       98   116      264    -


 205        0.01      CHLOROBENZAMIDE    619567
 139     0.70  0.55    0.13          0.77  1.25     0.50  0.84
 155     0.38  0.30    0.07          0.42  0.68     0.27  0.46

 206        1.00      3,4-DICHLOROBENZALDEHYDE   6287383
 173     0.48  0.39    0.09          0.58  0.93     0.31  0.57
 174     0.32  0.26    0.06          0.39  0.62     0.21  0.34

 207        0.71      1,2,4-TRICHLOROBENZENE   120821
 145     0.34  0.26    0.06          0.40  0.63     0.22  0.36
 180     1.30  1.00    0.24          1.50  2.40     0.83  1.37

 208        0.56      2-BROMO-1-CHLOROBENZENE    694804
 190     0.78  0.61    0.14          0.85  1.38     0.55  0.92
 192     1.04  0.81    0.19          1.14  1.84     0.74  1.24

 209        0.87      1,2-DICHLORONAPHTHALENE 2050693
 161     0.44  0.34    0.08          0.50  0.78     0.28  0.46
 196     2.17  1.67    0.40          2.51  3.88     1.38  2.29

 210        0.77      1,2,4,5-TETRACHLOROBENZENE  95943
 214     1.18  0.90    0.22          1.29  2.09     0.84  1.40
 216     1.54  1.18    0.28          1.69  2.72     1.09  1.83

 211        0.65      P-DIBROMOBENZENE  106376
 234     0.68  0.52    0.12          0.77  1.23     0.41  0.67
 236     1.29  1.00    0.23          1.48  2.36     0.78  1.30

 212        0.93      4-BROMODIPHENYLETHER    6452499
 248     1.08  0.81    0.20          1.19  1.92     0.77  1.29
 250     1.13  0.88    0.21          1.26  2.04     0.82  1.37

 213        0.64      HEXACHLOROBENZENE    118741
 284     0.74  0.56    0.13          0.84  1.34     0.44  0.73
 286     0.60  0.46    0.11          0.68  1.08     0.36  0.59
```

```
          Internal/External Standard File for Cmpd Class # 8

Cmpd#     Recovery   Compound Name
           Std #62     Std #63
Mass      188    -     99    -


 205         0.01    CHLOROBENZAMIDE   619567
 139     0.05         0.76
 155     0.03         0.41

 206         1.00    3,4-DICHLOROBENZALDEHYDE   6287383
 173     0.04         0.57
 174     0.03         0.38

 207         0.71    1,2,4-TRICHLOROBENZENE   120821
 145     0.03         0.36
 180     0.10         1.36

 208         0.56    2-BROMO-1-CHLOROBENZENE    694804
 190     0.05         0.84
 192     0.07         1.12

 209         0.87    1,2-DICHLORONAPHTHALENE 2050693
 161     0.03         0.46
 196     0.17         2.27

 210         0.77    1,2,4,5-TETRACHLOROBENZENE  95943
 214     0.08         1.27
 216     0.11         1.66

 211         0.65    P-DIBROMOBENZENE  106376
 234     0.05         0.75
 236     0.10         1.45

 212         0.93    4-BROMODIPHENYLETHER    6452499
 248     0.07         1.17
 250     0.08         1.24

 213         0.64    HEXACHLOROBENZENE   118741
 284     0.06         0.82
 286     0.05         0.66
```

Table B-9. RMRs AND RECOVERIES FOR ESSA COMPOUNDS

Class No. 9

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
64	d_{13}-Heptanoic acid (internal)
65	d_5-Benzoic acid (internal)

MATRIX OF STANDARD ION RMRs

			Standard						
			4-Fluoro-2-iodotoluene		2-Fluorobiphenyl	d_{13}-Heptanoic acid methyl ester		d_5-Benzoic acid methyl ester	
Standard	Ion	Recovery	m/z 109	m/z 236	m/z 172	m/z 77	m/z 91	m/z 82	m/z 110
4-fluoro-2-iodotoluene	109	NA	-	.78	.29	.99	3.47	1.73	.87
	236	NA	1.28	-	.37	1.27	4.46	2.21	1.12
2-fluorobiphenyl	172	NA	3.44	2.68	-	3.42	11.96	5.94	3.00
d_{13}-heptanoic acid methyl ester	77	0.65	1.01	.79	.30	-	3.47	1.74	.88
	91	0.65	.29	.23	.084	.29	-	.50	.25
d_5-benzoic acid methyl ester	82	0.92	.58	.45	.17	.58	2.00	-	.51
	110	0.92	1.15	.90	.34	1.14	3.97	1.98	-

```
          Internal/External Standard File for Cmpd Class # 9

Cmpd#     Recovery    Compound Name
           Std # 2       Std # 3        Std #64        Std #65
Mass      109   236    172    -        77     91       82    110


 101        0.79      CHLOROACETIC   79118
  59     0.58  0.46    0.17            0.58  1.86     1.01  0.51
  77     0.24  0.19    0.07            0.24  0.76     0.41  0.21

 102        0.82      VALERIC   109524
  74     0.58  0.45    0.17            0.58  1.84     1.00  0.51
  87     0.18  0.14    0.06            0.18  0.59     0.32  0.16

 103        0.01      MERCAPTOPROPIONIC
  61     0.24  0.18    0.07            0.23  0.81     0.41  0.21
 120     0.14  0.11    0.04            0.14  0.49     0.25  0.13

 104        0.01      MALONIC   141822
  59     0.63  0.49    0.18            0.63  2.03     1.10  0.55
 101     0.47  0.37    0.14            0.47  1.51     0.82  0.41

 105        0.01      SUCCINIC   110156
  55     0.42  0.33    0.12            0.41  1.44     0.72  0.36
 115     0.84  0.65    0.24            0.83  2.88     1.44  0.73

 106        0.92      BENZOIC   65850
  77     0.74  0.58    0.22            0.74  2.58     1.28  0.65
 105     1.43  1.11    0.42            1.41  4.94     2.45  1.24

 107        0.73      DICHLOROACETIC   79436
  59     0.82  0.64    0.24            0.82  0.39     1.42  0.72
  83     0.32  0.25    0.09            0.32  0.23     0.55  0.28

 108        0.91      P-TOLUIC   99945
 119     1.84  1.43    0.53            1.82  6.35     3.17  1.60
 150     0.66  0.51    0.19            0.66  2.28     1.14  0.58

 109        0.85      BROMOACETIC    79083
  59     0.12  0.09    0.24            0.12  0.39     0.21  0.10
  93     0.07  0.05    0.09            0.07  0.23     0.12  0.06

 110        0.82      N-OCTANOIC    124072
  74     1.61  1.26    0.47            1.60  5.56     2.78  1.40
  87     0.61  0.48    0.18            0.61  2.12     1.06  0.53

 111        0.90      O-METHOXYBENZOIC     579759
  77     0.47  0.36    0.14            0.46  1.61     0.80  0.41
 135     1.06  0.81    0.31            1.05  3.65     1.82  0.92

 112        0.88      2-NITRO-P-CRESOL  119335
  91     0.40  0.31    0.12            0.40  1.38     0.69  0.35
 167     0.42  0.33    0.12            0.41  1.44     0.72  0.36

 113        0.91      O-CHLOROBENZOIC  118912
 139     1.43  1.11    0.41            1.41  4.94     2.46  1.24
 170     0.42  0.33    0.12            0.41  1.45     0.72  0.36
```

```
             Internal/External Standard File for Cmpd Class # 9

Cmpd#    Recovery    Compound Name
          Std # 2      Std # 3       Std #64       Std #65
Mass      109   236    172    -       77    91      82   110


  114       0.85     N-NONANOIC   112050
   74    1.73  1.35   0.50           1.72  5.98    2.99  1.51
   87    0.75  0.58   0.22           0.74  2.58    1.29  0.65

  115       0.88     2,4-DICHLOROPHENOL  120832
  161    0.77  0.60   0.22           0.77  2.67    1.33  0.67
  176    0.90  0.70   0.26           0.89  3.10    1.54  0.78

  116       0.80     TRICHLOROACETIC  76039
  117    0.12  0.09   0.03           0.12  0.39    0.21  0.11

  117       0.88     NITROBENZOIC-(P)   62237
  150    0.00  0.00   0.00           0.00  0.02    0.01  0.00
  181    0.12  0.09   0.03           0.12  0.39    0.20  0.10

  118       0.94     NAPHTHOIC-2  93094
  127    0.78  0.61   0.23           0.78  2.70    1.35  0.68
  155    1.05  0.82   0.31           1.05  3.64    1.81  0.92

  119       0.87     N-DECANOIC   334485
   74    1.92  1.50   0.56           1.91  6.72    3.32  1.68
   87    0.91  0.71   0.26           0.90  3.16    1.56  0.79

  120       0.01     2,4-DINITROPHENOL  51285
  168    0.09  0.07   0.03           0.09  0.31    0.16  0.08
  198    0.13  0.10   0.04           0.13  0.41    0.22  0.11

  121       0.01     3,4-DICHLOROBENZOIC      51445
  173    0.15  0.11   0.04           0.15  0.51    0.25  0.13
  204    0.04  0.03   0.01           0.04  0.14    0.07  0.04

  122       0.93     2,3,6-TRICHLOROPHENOL    933755
  169    0.42  0.32   0.12           0.41  1.46    0.72  0.36
  212    0.68  0.53   0.20           0.68  2.39    1.17  0.59

  123       1.06     LAURIC  143007
   74    2.23  1.69   0.65           2.23  7.74    3.87  1.95
   87    1.21  0.92   0.35           1.20  4.17    2.08  1.05

  124       1.10     2,4-DICHLOROPHENOXYACETIC      94757
  175    0.47  0.36   0.14           0.46  1.61    0.80  0.41
  199    0.67  0.52   0.20           0.67  2.33    1.16  0.59

  125       0.90     MYRISTIC    544638
   74    3.12  2.43   0.91           3.10 10.80    5.38  2.72
   87    1.86  1.45   0.54           1.85  6.45    3.21  1.62

  126       0.99     2,4,5-TRICHLOROPHENOXYACETIC       93765
  233    0.53  0.42   0.16           0.53  1.85    0.92  0.46
  270    0.23  0.18   0.07           0.23  0.79    0.39  0.20
```

```
          Internal/External Standard File for Cmpd Class # 9

Cmpd#   Recovery   Compound Name
         Std # 2      Std # 3      Std #64       Std #65
Mass    109   236    172    -      77     91      82    110


  127     0.89     PALMITIC  57103
  74   2.86  2.23  0.83          2.85  9.85   4.93  2.49
  87   1.78  1.39  0.52          1.77  6.12   3.07  1.55

  128     1.00     PENTACHLOROPHENOL  87865
 265   0.50  0.39  0.14          0.49  1.71   0.85  0.43
 280   0.47  0.37  0.14          0.47  1.68   0.81  0.41

  129     0.63     OLEIC    112801
  55   0.45  0.35  0.14          0.47  1.52   0.81  0.41
  69   0.31  0.24  0.09          0.32  1.04   0.56  0.28
```

Table B-10. RMRs AND RECOVERIES FOR VOSA COMPOUNDS

Class No. 10

Standard ID No.	Standard Name
3	2-Fluorobiphenyl (external)
67	d_7-Butyric acid (internal)

MATRIX OF STANDARD ION RMRs

			Standard		
			2-Fluorobiphenyl	d_7-Butyric Acid Benzyl Ester	
Compound	Ion	Recovery	m/z 172	m/z 50	m/z 109
2-Fluorobiphenyl	172	NA	-	8.10	2.63
d_7-Butyric Acid	50	1.00	.13	-	.33
Benzyl Ester	109	1.00	.39	3.06	-

```
              Internal/External Standard File for Cmpd Class #10

 Cmpd#    Recovery   Compound Name
           Std # 3     Std #67
 Mass     172    -      50   109


  100       0.74     2-METHYLCYCLOPROPANE CARBOXYLIC ACID
   83    0.38         2.94  0.95
  190    0.07         0.56  0.18

  101       0.78     2-METHYLBUTENOIC ACID
   83    0.28         2.18  0.71
  190    0.03         0.21  0.07

  102       0.72     DIMETHYLACRYLIC ACID     541479
   83    0.54         4.14  1.34
  190    0.04         0.28  0.09

  103       0.74     2-METHYLBUTYRIC ACID     623427
  108    0.17         1.28  0.42
  192    0.11         0.84  0.27

  104       0.88     ISOVALERIC ACID   503742
  108    0.28         2.18  0.71
  192    0.07         0.50  0.16

  105       0.61     2-HEXENOIC ACID
   97    0.36         2.80  0.91
  204    0.02         0.14  0.05

  106       0.61     3-HEXENOIC ACID
  144    0.08         0.64  0.21
  204    0.01         0.06  0.02

  107       0.47     CYCLOPENTYLACETIC ACID
  108    0.29         2.26  0.73
  218    0.02         0.20  0.07

  108       0.01     ACETIC ACID   64197
  108    0.28         2.24  0.73
  150    0.08         0.67  0.22

  109       0.90     ACRYLIC ACID  79107
   55    0.08         0.66  0.21
  102    0.04         0.28  0.09

  110       0.01     PROPIONIC ACID  79094
  108    0.30         2.36  0.77
  104    0.09         0.73  0.24

  111       0.57     METHACRYLIC ACID  79414
   91    0.28         2.25  0.73
  131    0.17         1.33  0.44

  112       0.77     CROTONIC ACID   3724650
   69    0.36         2.87  0.93
   91    0.24         1.89  0.61
```

```
              Internal/External Standard File for Cmpd Class #10

Cmpd#     Recovery    Compound Name
           Std # 3       Std #67
Mass      172    -       50   109


 113        0.57      N-BUTYRIC ACID    107926
 108     0.37          2.93  0.96
 178     0.09          0.70  0.23

 114        0.42      ISOBUTYRIC ACID     79312
  91     0.44          3.49  1.13
 178     0.10          0.80  0.26

 115        0.75      N-PENTANOIC ACID 109524
  57     0.11          0.84  0.27
  91     0.39          3.09  1.01

 116        0.60      N-HEXANOIC ACID  142621
  43     0.12          0.96  0.31
  91     0.48          3.79  1.23

 117        0.57      2-ETHYLBUTRIC ACID 88095
  71     0.15          1.19  0.39
  91     0.33          2.65  0.36

 118        0.48      N-HEPTANOIC ACID 111148
  43     0.15          1.21  0.39
  91     0.51          4.02  1.31

 119        0.46      N-OCTANOIC ACID 124072
  91     0.66          5.22  1.70
 105     0.36          2.83  0.92

 120        0.01      N-NONANOIC ACID  112050
  91     0.46          3.64  1.19
  92     0.14          1.09  0.36

 121        0.32      CYCLOHEXANE CARBOXYLIC ACID   98895
  55     0.20          1.62  0.53
  91     0.46          3.67  1.19

 122        0.37      CYCLOHEXYL ACETIC ACID    5292217
  81     0.40          3.17  1.03
  91     0.69          5.50  1.79
```

Table B-11. RMRs AND RECOVERIES FOR NOVA COMPOUNDS

Class No. 11	
Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
66	d_7-Naphthalene sulfonic acid (internal)

MATRIX OF STANDARD ION RMRs

Compound	Ion	Recovery	d_7-Naphthalenesulfonic acid methyl ester		2-Fluorobiphenyl	4-Fluoro-2-iodotoluene		d_{25}-dodecylphosphonic acid dimethyl ester
			m/z 134	m/z 229	m/z 172	m/z 109	m/z 236	m/z 129
d_7-naphthalenesulfonic acid methyl ester	134	1.10	-	1.71	.23	.81	.63	.63
	229	1.10	.59	-	.14	.47	.37	.14
2-fluorobiphenyl	172	NA	4.46	7.62	-	3.43	2.67	.99
4-fluoro-2-iodotoluene	109	NA	1.31	2.24	.29	-	.78	.29
	236	NA	1.69	2.88	.38	1.29	-	.37

```
              Internal/External Standard File for Cmpd Class #11

Cmpd#    Recovery   Compound Name
          Std # 2     Std # 3      Std #66
Mass     109   236    172    -     134   229


 100       0.01     THIOGLYCOLIC     68111
  91    0.08  0.06   0.02          0.11  0.20
 105    0.39  0.30   0.12          0.53  0.91

 101       0.28     SUCCINIC   110156
  55    0.21  0.17   0.06          0.29  0.49
 115    0.42  0.32   0.12          0.56  0.96

 102       1.10     BENZENESULFONIC      98113
  77    0.98  0.76   0.29          1.25  2.13
 172    0.34  0.27   0.10          0.44  0.78

 103       0.68     M-NITROBENZOIC   121926
 104    0.07  0.05   0.02          0.09  0.16
 150    0.25  0.20   0.07          0.34  0.58

 104       1.40     BENZENEPHOSPHONIC    1779482
  91    0.46  0.36   0.13          0.59  1.01
 185    0.45  0.35   0.13          0.57  0.98

 105       0.72     P-TOLUENESULFONIC  104154
  91    1.16  0.91   0.34          1.48  2.52
 186    0.48  0.37   0.14          0.60  1.03

 106       0.55     TEREPHTHALIC     100210
 163    1.85  1.44   0.54          2.37  4.04
 194    0.44  0.34   0.13          0.56  0.96

 107       0.42     3,4-DICHLOROBENZOIC     51445
 173    0.69  0.54   0.20          0.92  1.56
 204    0.20  0.16   0.06          0.26  0.45

 108       0.92     P-CHLOROBENZENESULFONIC      98668
 111    0.59  0.46   0.17          0.75  1.28
 206    0.24  0.19   0.07          0.31  0.52

 109       1.10     2-NAPHTHALENESULFONIC     120183
 127    0.87  0.68   0.25          1.08  1.82
 222    0.52  0.40   0.15          0.64  1.08

 110       0.61     2,4,5-TRICHLOROPHENOXYACETIC  93765
 233    0.46  0.36   0.13          0.58  1.00
 270    0.20  0.15   0.06          0.25  0.43

 111       0.62     PENTACHLOROPHENOL    87865
 265    0.50  0.39   0.14          0.01  0.01
 280    0.47  0.37   0.14          0.01  0.01

 112       0.01     OLEIC  112801
  55    0.35  0.27   0.10          0.45  0.76
  69    0.24  0.19   0.07          0.31  0.54
```

Table B-12. RMRs AND RECOVERIES FOR SAM-PT COMPOUNDS

Class No. 12

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene (external)
3	2-Fluorobiphenyl (external)
68	d_9-Butylamine (internal)

MATRIX OF STANDARD ION RMRS

			Standard				
			4-Fluoro-2-iodotoluene		2-Fluorobiphenyl	d_9-Butylamine	
Compound	Ion	Recovery	109	236	172	210	212
4-fluoro-2-iodotoluene	109	NA	-	.78	.30	4.16	10.68
	236	NA	1.28	-	.39	5.32	13.68
2-fluorobiphenyl	172	NA	3.31	2.58	-	13.74	35.3
d_9-Butylamine	210	0.75	.24	.19	.073	-	2.58
	212	0.75	.094	.073	.028	.39	-

```
             Internal/External Standard File for Cmpd Class #12

Cmpd#    Recovery   Compound Name
          Std # 2      Std # 3       Std #68
Mass     109   236    172    -       210   212


  100       0.75      ALLYL AMINE  107119
   41    0.09  0.07    0.03            0.37  0.95
  207    0.04  0.03    0.01            0.15  0.39

  101       0.75      N-BUTYLAMINE    109739
  190    0.08  0.06    0.03            0.83  2.15
  208    0.20  0.16    0.06            0.84  4.11

  102       0.76      ISOBUTYLAMINE     78819
  208    0.38  0.30    0.12            1.60  4.11
  209    0.11  0.09    0.03            0.47  1.21

  103       0.77      SEC-BUTYLAMINE      13952846
  222    0.28  0.22    0.09            1.16  2.99
  236    0.05  0.04    0.01            0.20  0.52

  104       0.75      T-BUTYLAMINE     75649
   57    0.48  0.38    0.15            2.01  5.18
  236    0.30  0.23    0.09            1.25  3.22

  105       0.74      N-HEXYLAMINE   111262
  208    0.19  0.15    0.06            0.80  2.07
  250    0.22  0.17    0.07            0.92  2.36

  106       0.74      CYCLOHEXYLAMINE  108918
   55    0.17  0.13    0.05            0.69  1.78
  194    0.10  0.08    0.03            0.44  1.12

  107       0.75      2-ETHYLHEXYLAMINE   104756
  208    0.23  0.18    0.07            0.97  2.49
  278    0.20  0.15    0.06            0.82  2.11

  108       0.75      BENZYLAMINE       100469
   91    0.33  0.26    0.10            1.36  3.49
   92    0.08  0.06    0.02            0.32  0.82

  109       0.73      ETHYLENE DIAMINE  107153
  208    0.05  0.04    0.02            0.22  0.57
  223    0.04  0.04    0.01            0.19  0.48

  110       0.75      TRIBUTYLAMINE     102892
  100    0.48  0.38    0.15            2.02  5.18
  142    1.71  1.31    0.52            6.98 17.91
```

Table B-13. RMRs AND RECOVERIES FOR SAM-S COMPOUNDS

Class No. 13

Standard ID No.	Standard Name
2	4-Fluoro-2-iodotoluene
3	2-Fluorobiphenyl
70	N-Ethyl-2-fluorobenzylamine

MATRIX OF STANDARD ION RMRs

			Standard				
			4-Fluoro-2-Iodotoluene		2-Fluorobiphenyl	N-Ethyl-2-Fluorobenzylamine	
Compound	Ion	Recovery	m/z 109	m/z 236	m/z 172	m/z 109	m/z 318
4-Fluoro-2-Iodotoluene	109	NA	-	0.77 (8)[a]	1.28 (1)	0.27 (6)	1.13 (26)
	236	NA	1.34 (1)	-	0.24 (2)	0.37 (6)	1.52 (27)
2-Fluorobiphenyl	172	NA	1.23 (9)	2.43 (8)	-	0.83 (8)	3.57 (26)
N-Ethyl-2-Fluorobenzylamine	109	1.00	4.00 (1)	3.11 (7)	0.32 (0)	-	4.53 (27)
	318	1.00	0.77 (1)	0.60 (6)	0.42 (2)	0.20 (10)	-

---

[a] Coefficient of variation for triplicate determinations are given in parenthesis.

```
            Internal/External Standard File for Cmpd Class #13

Cmpd#    Recovery    Compound Name
          Std # 2      Std # 3        Std #70
Mass     109   236    172     -      109   318


 100       0.82      DIALLYLAMINE   124027
 181    1.73  1.83    0.75           0.60  2.70
 250    0.68  0.57    0.24           0.19  0.80

 101       0.64      DIPROPYLAMINE  142847
 181    2.02  1.57    0.56           0.57  2.44
 252    1.80  1.47    0.60           0.48  2.09

 102       0.45      PIPERIDINE   110894
 181    1.66  1.32    0.55           0.44  1.93
 264    1.13  0.91    0.37           0.30  1.31

 103       0.15      MORPHOLINE   110918
 181    2.45  1.94    0.79           0.65  2.82
 267    0.42  0.34    0.14           0.11  0.49

 104       0.45      METHYLPIPERIDINE(2)  626675
 181    2.68  2.13    0.88           0.71  3.09
 264    2.88  2.28    0.93           0.76  3.08

 105       0.45      DIBUTYLAMINE  111922
 181    0.42  0.31    0.12           0.10  0.98
 195    0.15  0.12    0.05           0.04  0.99

 106       0.40      DIMETHYLPIPERIDINE(2,6)    671363
 224    0.85  0.66    0.27           0.22  0.97
 266    1.76  1.38    0.56           0.46  2.00

 107       0.01      DIETHYLAMINE   109897
 181    0.75  1.19    0.48           0.39  1.94
 253    0.35  0.06    0.02           0.02  0.11

 108       0.01      DIBENZYLAMINE 103491
  91    6.04  4.88    2.00           1.60  6.91
 377    0.40  0.32    0.13           0.10  0.53
```

APPENDIX C

DESCRIPTION OF COMPUTER PROGRAM MASQUANT FOR PROCESSING DATA COLLECTED USING MAS

Description of the Computer Program MASQUANT for Processing and Editing Data Collected Using the Master Analytical Scheme

I. General

A computer program called MASQUANT has been written to carry out some of the basic calculations used to process data obtained using the Master Analytical Scheme. MASQUANT consists of approximately 2,000 lines of source code written in ANSI subset Fortran 77, which should make it operable on any computer capable of handling this language.

The program consists of a main routine and sixteen subroutines, which will be described in greater detail below. The program is written to be run interactively, with a continuing dialogue between the user and the computer. After all of the data are collected, a report giving the calculated concentration of each identified component is generated.

In order to use MASQUANT, three files need to be accessed from an external disk or tape. The files are organized in a sequential fashion, and are read or written to in this same manner. These files are 1) a file which contains calculated correction factors for RMRs, which can be applied to the library file, if desired; 2) a standard file consisting of internal and external standards, along with associated data including recovery factors and response factors; and 3) a file, written in the identical format as file 2, consisting of data for "unknown" analytes. The compounds and standards are organized into 13 classes, consistent with the MAS Protocols. Detailed formats for the three files are given in this Appendix.

II. Description of the Operation of Individual Routines

(1) Main Program

The main program organizes the entire scheme and carries out a number of specific calculations internally. On initialization, it determines in what units the final results are to be reported, the name of the run, the data and the class of unknown being analyzed. It determines if system performance standards (SPS) are to be used in modifying the stored RMR values used in the analysis. It then proceeds to gather information about the external and internal standards to be used in the

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analysis. After the standards have been entered, the program determines which ion of each internal standard will be used in the calculation for each unknown. The protocol is briefly as follows: Each internal standard is examined in order. For each internal standard, one external standard is chosen for comparison. The external standard chosen is that standard whose relative retention time is closest to that of the internal standard. The amount of internal standard present is calculated two ways: directly from the amount specified by the user corrected for standard recovery (forward calculation) and by calculation using RMRs stored for the particular internal standard/external standard combination (backward calculation). If SPS has been specified, these RMRs are corrected according to the SPS protocol. Forward calcuation is carried out once and the reverse calculation is carried out four times for each of the possible combination of ions of internal and external standards (2 x 2). The internal standard ion chosen is that for which the weight corresponding to the reverse calculation is closest to that of the forward calculation.

A single ion for each internal standard is chosen in this manner, and then the unknowns are processed. Data for each individual unknown are collected and the concentration of that component is computed according to the formulas shown in the flow chart, using the internal standard which has been chosen as described previously. After all of the unknowns have been processed in this fashion, a report, showing the concentration of each unknown, is generated. At present the program can accommodate 50 unknowns in each pass. After each report is generated, the program restarts and the process can be repeated as often as desired.

(2) Subroutine BUGTAB

BUGTAB writes out a table of correction factors which are read in using subroutine TABLRW, or which are generated by program SPS. The internal standards and external standards are independently listed along with the appropriate correction factor.

(3) Subroutine DUPOUT

Subroutine DUPOUT checks the array of standard or unknown numbers for duplicates. The arrays must have previously been sorted in ascending sequence. If a duplicate is found, it is set equal to 10,000. Finally, the array is resorted, and the number of elements in the original array is reduced by the number of duplicate entries found.

(4) Subroutine ENTER

Subroutine ENTER is used to enter a series of numbers which are either internal standards, external standards, or unknowns. The subroutine is called four times in the program. It is called once by SPS, once for external standard entries, once for internal standard entries, and once for unknown entries. The numbers are entered using subroutine INPUT. Ten entries are permitted on each line, and the entire list of entries is terminated with a zero entry. The program also does range checks for each type of compound. External standard numbers may range from 1 to 49; internal standards from 51 to 99, and unknowns from 101 to 999. After the numbers are acquired, the list is sorted in ascending sequence and duplicates are removed.

(5) Subroutine FILERD

This subroutine reads data from either the standard file or the unknown file. Records are read sequentially from the beginning of the file until a match is found for the class number and the standard number. If the compound which is sought is not found, an error statement is issued; otherwise all of the file data including the compound name, molecular weight, recovery factor, ion masses, RMRs, etc. are returned for each compound sought.

(6) Subroutine GETRMR

This subroutine simply returns one chosen RMR from those present in the table. Parameters are passed to the subroutine which select the appropriate reference standard and the individual ion of the compound.

(7) Subroutine GTDATA

This subroutine queries the user to provide the relative retention time and on-column weight for a given substance. The subroutine has three entries: one for external standard, one for internal standard, and one for unknowns. The data are entered into the system by use of the subroutine INPUT. The program rejects zero values as entries.

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(8) Subroutine INPUT

INPUT is a modified version of a standard ANSI Fortran subroutine designed to permit field-free input for numeric data. The program has been altered for this application. Numbers can be entered into the first fifty columns of each line. Only one line of data can be entered by a single subroutine call. Numbers can be entered as integers or as floating point numbers containing a single decimal point. Delimiters between numbers are either a succession of blanks or a single comma. Besides numerals, commas, periods and blanks only the letters "R", "B", and the symbol "?" are allowed as entries. "R" returns a code which is used to restart the program; "B" is used to allow the user to back up in the program and repeat the previous section. A question mark is used to signal an error, and the entire line can then be re-entered. All other characters, including "+" and "-" are not allowed. Further details of this program are found in the source listings.

(9) Subroutine ISREP

Subroutine ISREP is a report routine which lists the data stored for internal standards. The variables listed are the standard number, its name, molecular weight, relative retention time, mass of ion used for computation, forward and backward calculated weights, and system response.

(10) Subroutine REPORT

REPORT writes out the final report for the analysis. In addition to reporting pertinent data for each run, each unknown is listed by name and number. The calculated concentration of each component is printed either in PPM (mg/l) or in PPB (μg/l).

(11) Subroutine RMRFIX

RMRFIX is a program whereby the RMR values listed for a particular internal standard or unknown are altered by multiplication by the appropriate correction factor which has been previously stored on a disk file. The subroutine is called twice: once to correct RMRs of internal standards, and once for unknowns. Although only a single RMR is used by the main program, for the sake of simplicity all of the RMRs for a given entry are altered.

(12) Subroutine SORTUP

Subroutine SORTUP is a very low level sort routine written to order integer numbers in ascending sequence. The algorithm used is a simple bubble sort. Every number is compared with every other. If the numbers are already in sequence, they are left without alteration. If they are out of sequence, the numbers are exchanged. Although this algorithm is not highly efficient, it is only used for a maximum of fifty entries, and a more sophisticated treatment was not warranted.

(13) Subroutine SPS

Subroutine SPS is a major subroutine which determines if system performance standards are to be employed in correcting the RMR values stored. If so, then a sequence is entered which calculates correction factors. The program is commented very completely in the source listing and by a flow chart. In brief, the program initially determines whether SPS processing is desired, whether a table exists, and whether or not an existing table should be left unaltered, deleted, or updated. The system allows storing only a single set of tables for one class of unknowns. If more than one class of unknowns are to be process using SPS, then the routine must be executed separately for each class.

The program works by obtaining weights, times, and responses for a series of not less than five ions. From these data a square matrix of RMRs are calculated, i.e., the RMR of each ion is calculated with respect to every other ion entered. Then, the RMRs permanently stored on disk or tape in the file for a single ion are compared with those just calculated, making use of a simple linear regression through the origin. The slope of each regression line is then stored as the correction factor for each ion. The correction factors are then written onto disk for permanent storage (until the subroutine SPS is run again).

(14) Subroutine SPSCHK

Subroutine SPSCHK is used to test entries made by the user under SPS protocol to make sure that there is a table entry stored for each ion reported. This subroutine is executed twice during the course of the program.

(15) Subroutine SYSRES

SYSRES is a data entry subroutine used to have the user enter system responses for a particular compound. The program already knows the ions for which responses are desired, and prompts the user to respond making use of the subroutine INPUT.

(16) Subroutine TABLRW

Subroutine TABLRW is used to communicate between the main program and the SPS table of correction factors. It can be used either to read the table or to write new data onto the table. In the read mode, the subroutine checks to see whether a table is or is not present for the class requested, and returns either the data or an appropriate return code to indicate that a table is absent.

(17) Subroutine YON

Subroutine YON is used to handle alphabetic answers to questions. If the first character typed is a "Y" or an "N", the subroutine returns an appropriate code. In addition, the subroutine recognizes an "R" character, a "B", and a "?". The R and B are used by the calling program for a system restart or backspace, respectively, and a question mark allows the user to re-enter his answer.

FORMAT OF
INTERNAL/EXTERNAL STANDARD FILE AND UNKNOWN
FOR MASTER ANALYTICAL SCHEME

1. Entries (records) in file are ordered by:

   1) class
   2) compound number
   3) ion mass

2. Each entry occupies of 1 or 2 records depending on the number of ions catalogued.

3. DCB=(RECFM=FB,LRECL=440,BLKSIZE=3960), UNIT = 7(IS and XS), 8(Unk)

   A. FIXED PORTION OF RECORD

Description	Format	First Column	Last Column	Byte Length
1) COMPOUND NAME.	36A2	1	72	72
2) BLANK	5X	73	77	5
3) NAME LENGTH	I3	78	80	3
4) MOL. WT.	I4	81	84	4
5) BLANK	2X	85	86	2
6) CPD. NUMBER	I4	87	90	4
7) CPD. CLASS	I2	91	92	2
8) MASS OF ION	I4	93	96	4
9) RECOVERY	F4.2	97	100	4
10) BLANK	1X	101	101	1
11) TYPE FLAG (1-IS; 2-XS; 3-?)	I1	102	102	1
12) NO. OF IONS (1 OR 2)	I1	103	103	1
13) ION NUMBER (1 OR 2)	I1	104	104	1
14) RECORD NUMBER	I4	105	108	4
15) NO. OF STDS. W/RMRs	I2	109	110	2
16) BLANK	10X	111	120	10

B. VARIABLE PORTION

Description	Format	Bytes	Standard Number (1)		(2)		(3)		(4)	
			FB	LB	FB	LB	FB	LB	FB	LB
ST. NO.	I2	2	121	122	141	142	161	162	181	182
ST. FLG. (1-XS; 2-IS)	I1	1	123	123	143	143	163	163	183	183
NO. OF STD. IONS (1 OR 2)	I1	1	124	124	144	144	164	164	184	184
ST. MASS 1	I3	3	125	127	145	147	165	167	185	187
RMR 1	F5.2	5	128	132	148	152	168	172	188	192
ST. MASS 2	I3	3	133	135	153	155	173	175	193	195
RMR 2	F5.2	5	136	140	156	160	176	180	196	200

Description	Format	Bytes	(5)		(6)		(7)		(8)	
ST. NO.	I2	2	201	202	221	222	241	242	261	262
ST. FLG. (1-XS; 2-IS)	I1	1	203	203	223	223	243	243	263	263
NO. OF STD. IONS (1 OR 2)	I1	1	204	204	224	224	244	244	264	264
ST. MASS 1	I3	3	205	207	225	227	245	247	265	267
RMR 1	F5.2	5	208	212	228	232	248	252	268	272
ST. MASS 2	I3	3	213	215	233	235	253	255	273	275
RMR 2	F5.2	5	216	220	236	240	256	260	276	280

Description	Format	Bytes	(9)		(10)		(11)		(12)	
ST. NO.	I2	2	281	282	301	302	321	322	341	342
ST. FLG. (1-XS; 2-IS)	I1	1	283	283	303	303	323	323	343	343
NO. OF STD. IONS (1 OR 2)	I1	1	284	284	304	304	324	324	344	344
ST. MASS 1	I3	3	285	287	305	307	325	327	345	347
RMR 1	F5.2	5	288	292	308	312	328	332	348	352
ST. MASS 2	I3	3	293	295	313	315	333	335	353	355
RMR 2	F5.2	5	296	300	316	320	336	340	356	360

Description	Format	Bytes	(13)		(14)		(15)		(16)	
ST. NO.	I2	2	361	362	381	382	401	402	421	422
ST. FLG. (1-XS; 2-IS)	I1	1	363	363	383	383	403	403	423	423
NO. OF STD. IONS (1 OR 2)	I1	1	364	364	384	384	404	404	424	424
ST. MASS 1	I3	3	365	367	385	387	405	407	425	427
RMR 1	F5.2	5	368	372	388	392	408	412	428	432
ST. MASS 2	I3	3	373	375	393	395	413	415	433	435
RMR 2	F5.2	5	376	380	396	400	416	420	436	440

FORMAT OF CORRECTION FACTOR TABLE FOR SYSTEM PERFORMANCE STANDARDS MASTER ANALYTICAL SCHEME

DCB=(RECFM=FB,LRECL=80,BLKSIZE=800), UNIT = 6

FIRST CARD DESCRIPTION

	Format	Bytes	First Column	Last Column
1. TABLE FLAG O-NO TABLE, 1-TABLE	I1	1	1	1
2. TABLE CLASS	I2	2	2	3
3. NO. OF STDS. (NTST)	I2	2	4	5
4. DATE	4A2	8	6	13

SUBSEQENT CARDS (NTST IN NUMBER)

	Format	Bytes	First Column	Last Column
1. STANDARD NUMBER	I3	3	1	3
2. INT/EXT FLAG (1 OR 2)	I1	1	4	4
3. NO. OF FACTORS (1 OR 2)	I1	1	5	5
4. MASS 1	I3	3	6	8
5. FACTOR 1	F5.4	5	9	13
6. MASS 2	I3	3	14	16
7. FACTOR 2	F5.4	5	17	21

TAPE DOCUMENTATION

The tape RA1375 was written in IBM standard label format in EBCDIC at 1600 B.P.1. The order, names, and contents of the data sets residing on the tape are as follows:

1) EPAQNT.CARD3.STDS

   Card image data for a single test class of standards for primary input file for the program ADD(s).

2) EPAQNT.CLASS3.STDS

   Test data set to be used as standard file input to MASQNT (11). This file can be generated by using ADD(5) with (1) as primary input.

3) EPAQNT.CARD3.ANLS

   Card image data for a single test class of analytes for primary input file for the program ADD(5).

4) EPAQNT.CLASS3.ANLS

   Test data set to be used as analyte file input to MASQNT (11). This file can be generated by using ADD(5) with (3) as primary input.

5) EPAQNT.ADD.SOURCE

   This file comprises the card image source code for the data base creation program ADD. See data base management documentation for input and output file numbers and formats.

6) EPAQNT.REPORT.SOURCE

   This file comprises the card image source code for the listing generation program REPORT. See data base management documentation for input and output file numbers and formats. Can be tested using either (2) or (4) as input.

7) EPAQNT.EDIT.SOURCE

This file comprises the card image source code for the data base modification program EDIT. The sample run can be reproduced by using (8) as control card input and (2) as primary input file. See data base management documentation for input and output file numbers and formats.

8) EPAQNT.EDIT.CNTLCARD

This file comprises card images which are to be used as control cards for EDIT (7) along with (2) in generating a test run.

9) EPAQNT.DELETE.SOURCE

This file comprises the card image source code for the program DELETE. The sample DELETE run can be produced using (10) as control cards and (1) as a primary input file. See data base management documentation for input and output file numbers and formats.

10) EPAQNT.DELETE.CNTLCARD

This file comprises card images which are to be used as control cards for DELETE (9) along with (2) in generating a test run.

11) EPAQNT.MASQNT.SOURCE

This file contains the card image source of the revised MASQNT. Sample analyte, standards, and table files are (4), (2), and (12) respectively.

12) EPAQNT.SPS.TABLES

This is a copy of the System Performance Standards tables used in the sample run of MASQNT.

A copy of a successful run for each of the four data base management programs was included. It should be possible to duplicate the same output on another machine with the documentation of each program being used and the appropriate combination from the above twelve tape datasets. Perhaps the easiest way to create a new MASQNT data base is to assign standard and analyte IDs according to the ADD documentation, fill out copies of the entry forms provided, and use a combination of the ADD, REPORT, and the editor of the particular machine being used. A sample of blank entry forms for ADD is provided herein.

MASQNT

This second version of MASQNT uses the same fortran unit numbers for input/output as the first;

Unit - User Input
Unit 3 - User Output
Unit 6 - System Performance Standard correction tables
Unit 7 - Standard Database
Unit 8 - Analyte Database

The protocol class names and their corresponding numbers are as follows:

1. Purge and Trap (VO)
2. Elevated Temperature Purge and Trap (NEWS)
3. Batch Liquid-Liquid Partitioning for pH 8 Extractables/ No fractionation (WABN- BLLE)
4. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 1 (WABN)
5. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 2 & 3 (WABN)
6. Batch L-L Partitioning for pH 8 Extractables/Fraction No. 3 (WABN)
7. Flow-Under L-L Partitioning for pH 8 Extractables (WABN-FU)
8. Accumulator Column for pH 8 Extractables (WABN-SC)
9. Batch L-L Partitioning (pH 1) for Acid Extractables (ESSA)
10. Anion Ion-Exchange/Distillation for short chain acids (VOSA)
11. Anion Ion-Exchange for strong acids (NOVA)
12. Cation Ion-Exchange for Primary and Tertiary Amines (SAM-PT)
13. Cation Ion-Exchange for Secondary Amines (SAM-S)

Data Base Management Programs For MASQNT

The data base management system for the master scheme consists of four programs: ADD, DELETE, REPORT, and EDIT. All of the programs are written in ANS1 Fortran and are intended to operate in a batch environment. The data base used by MASQNT consists of two files: a standard file which contains the RMR's of standards versus each other and an analyte file which contains RMR's of analytes versus standards. The format of the standard and analyte files are the same and any of the four programs can be used on either file. While the programs should be protable they do not by themselves furnish the capability of modifying the MASQNT data base. The sort utility of the machine being used must be used in preprocessing or postprocessing steps. The control cards to three (DELETE, REPORT, and EDIT) must be sorted in a particular sequence as well as the output files generated by three programs (ADD, REPORT, and EDIT). Also some file handling utilities have to be used in conjunction with the programs which modify the files (ADD, EDIT, and DELETE). These programs use the original data file (standard or analyte) and card images as input and write the updated output to a different file. The renaming, deleting, backup, and changing to the new input file for MASQNT must be done by the user with utility programs on the machine these programs are being run on.

REPORT

The program REPORT produces a formatted listing of the files used by MASQNT from card images specified by the user. REPORT is used to generate listings of the data base, to verify the correctness of new entries made into the data base by ADD.

REPORT reads the MASQNT file from unit 6 and writes a listing output to unit 3. The control cards are read from unit 1 and must be ordered by ascending class numnber (card columns 15-16) and by ascending compound number (card columns 17-20) within class number. Error messages concerning control cards are written to unit 4. Two types of controls cards are recognized by REPORT: LIST and ALL. The ALL card is used to generate a listing of the entire file. All that is needed to generate a complete file listing specific entries in the file when a complete printout is not desired. A typical use of the LIST option would be to verify the correctness of changes (on a limited number of entries) made by the program EDIT.

```
LIST      26   8    63
LIST    1530   9     3
LIST      58   9   761
LIST      61   9   772
```

Format of Control Cards for Report:

	Beginning Column	Ending Column	Field Contents
LIST	1	4	LIST
	11	14	Record # of Compound (right justified)
	15	16	Class # of Compound (right justified)
	17	20	Compound # (right justified)
	21	21	Ion #
ALL	1	3	ALL

The field in column 21 of the LIST card is used for printing out individual ions for a compound entry, i.e., a 1 coded in column 21 will cause the program to list the first ion only and an 2 will cause the program to list the second ion only. Leaving column 21 blank will cause the program to list all ions for the given compound.

The numeric entries in the field columns 11-14, 15-16, and 17-20 must be right justified. The control cards must also appear in order class # and compound # within class #.

Since the LIST card is intended for use with only a few specific entries and since the ALL card can always be used to print the entire file, the number of control cards for REPORT should be limited, thereby making it easy for the user to enter control cards in the proper order. However, in the event ov a large number of LIST cards it should be possible to order the cards in a prior step with the sort program of the particular machine being used.

DELETE

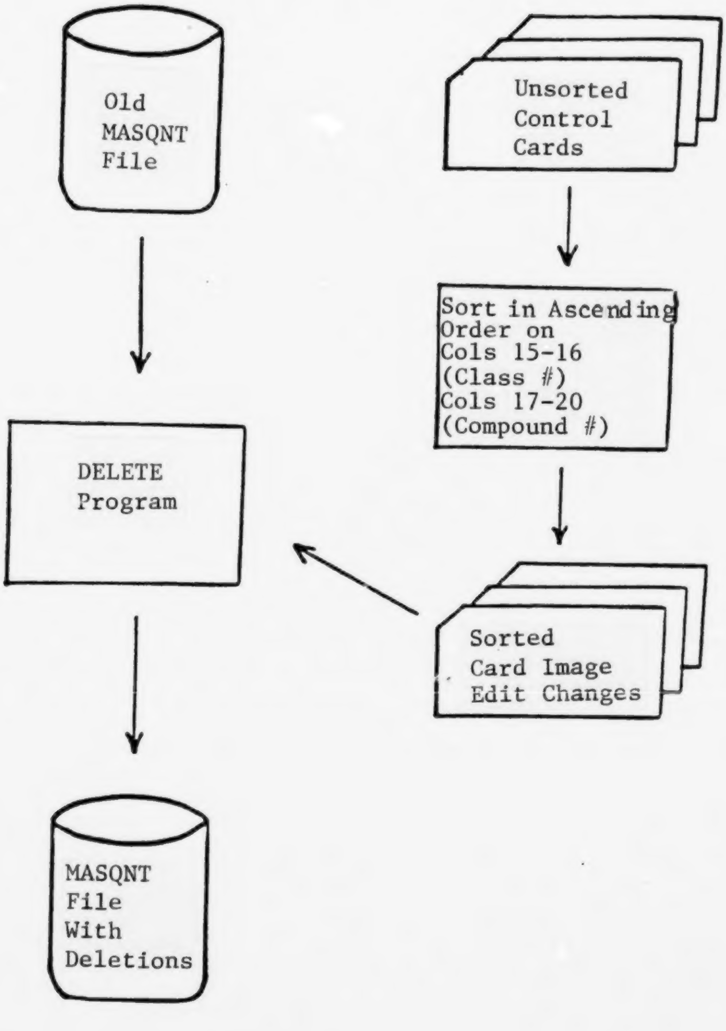
The program DELETE is used to eliminate entries from the data base which are no longer used or which have been found to have been entered incorrectly. DELETE reads control cards specifying which compounds are to be deleted from unit 1, reads the input file from unit 7, and writes the output file to unit 8. Error messages and messages telling which entries were deleted are written to unit 3. Each run of DELETE is in a sense tentative because the original file is left intact. If the user is not satisfied with the error messages returned by the program, he can simply alter the control cards and run DELETE again using the same input and output files. When a DELETE run without error messages is obtained the user can then finalize the deletions by scratching the input file and renaming the output file to the old input file name with the utility programs of his particular machine. ONly one type of control card is recognized by DELETE, the 'DEL' card which is specified by coding DEL in card columns 1-3. The user enters one DEL card for each compound to be deleted from the file. The program expects the cards to be sorted in order of ascending class number and by ascending compound number within class number. Having the cards out of order will cause DELETE to issue an error message. In the event that many entries are to be deleted, it may be advantageous to sort the control cards with a utility program prior to running DELETE.

The format of the DEL cards is as follows:

Beginning Column	Ending Column	Field Contents
1	3	DEL
11	14	Record # of 1st Compound Ion (right justified)
15	16	Class # of Compound (right justified)
17	20	Compound # (right justified)

```
DEL      1010004
DEL      3010052
DEL     11020057
```

As with REPORT the numeric entries in the field columns 11-14, 15-16 and 17-20 are all right justified. Also as with REPORT, the control cards should be entered in order of ascending class # and compound # within class #.


Old
MASQNT
File
Unsorted
Control
Cards
Sort in Ascending
Order on
Cols 15-16
(Class #)
Cols 17-20
(Compound #)
DELETE
Program
Sorted
Card Image
Edit Changes
MASQNT
File
With
Deletions

Steps for DELETE Program

EDIT

The program edit is used to modify existing entries in either the standard or analyte files. The control cards are read from unit 1, the old data file is read from unit 7, and the new modified data file is written to unit 8. Messages from EDIT are written to unit 3, like DELETE and ADD, each run with EDIT is tentative because the original file is not modified. The EDIT program can be run as many times as needed until a correct output file is generated. The changes made by EDIT become final only when the input file is scratched. EDIT can be run on the standard file to modify RMR's of standards or on the analyte file to modify RMR's of analytes versus standards. EDIT recognizes three types of control cards: The CRMR card which modifies existing RMR's, the ASTD card which adds RMR's for new standards. The control cards to EDIT must appear in order of ascending class number (card columns 15-16), ascending compound number within class (card columns 17-20), and ascending ion # within compound (card column 21) in order for EDIT to work properly. As with DELETE and REPORT, the sort program of the particular machine may have to be used in the instance of a large number of cards. No sorting of the output file of EDIT is required.

The format of the CRMR is as follows:

Beginning Column	Ending Column	Field Contents
1	3	ADD
6	6	Number of Ions for Compound (1 or 2)
8	9	Number of Standards (1 to 16)
11	12	Class Number (see figure for permissable codes)
14	14	Type (1 to 3) 1 = External Standard 2 = Internal Standard 3 = Analyte
16	19	Mass of 1st compound ion
21	24	Mass of 2nd compound ion
26	29	Compound molecular weight
32	35	Recovery fraction for compound (Real fraction between 0.0 and 1.0)
37	39	Compound ID

The NAME card has only one item: The name of the compound being added which starts in column 6. The STD cards follow the ADD and NAME cards. Each STD card contains the RMR's for a given ion of the compound being added relative to a given standard. The number of ions permitted for a compound is either 1 or 2 and is coded in column 6 of the ADD card. The number of STD cards which are to follow for each ion is coded in columns 8-9 of the ADD card. The STD cards for the second ion - if the compound has two ions - follow the STD cards for the first. The items on a STD card and their respective fields are as follows:

Beginning Column	Ending Column	
1	3	STD
6	6	Ion Number (1 or 2)
8	9	Sequence Number of Standard within Ion (1 to 16)
11	12	Standard ID (Explained Below)
14	14	Standard Type (1 = External, 2 = Internal)
21	23	1st Standard Ion Mass
26	30	1st Standard RMR
32	34	2nd Standard Ion Mass
37	41	2nd Standard RMR

The format of the ASTD card is as follows:

Beginning Column	Ending Column	
1	4	ASTD
11	14	Record # of Compound
15	16	Class # of Compound
17	20	Compound #
21	21	Ion #
26	27	ID # of Standard within Record
29	29	Standard Type (1 = External, 2 = Internal)
31	33	Mass #1
35	39	RMR #1
41	43	Mass #2
45	49	RMR #2

The entries in columns 11-21 are used to locate the correct entry in the data base. The ID number for the standard should be consistent with the instructions to ADD. If there are already sixteen standards for the compound ion the program will print an error message with no change of the standard record.

The DSTD card accomplishes the reverse of the ASTD card - it is used to strike RMR references to standards which are no longer to be used and which have been deleted from the standards file.

The format of the DSTD card is as follow:

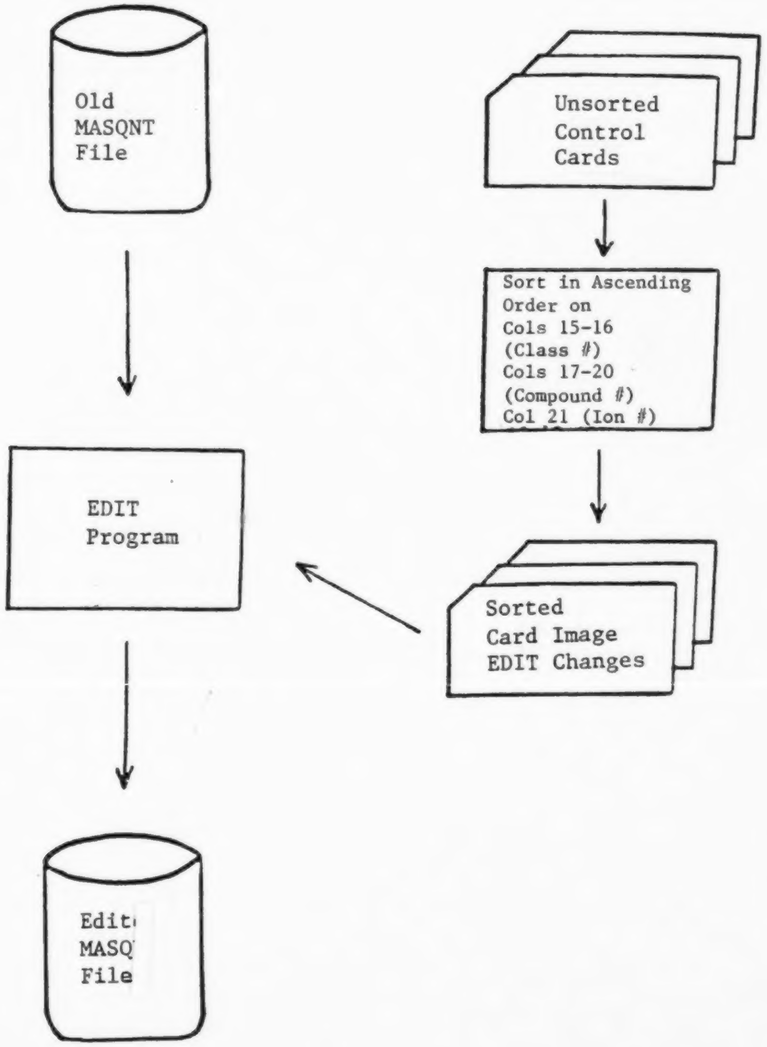
Beginning Column	Ending Column	
1	4	DSTD
11	14	Record # of Compound
15	16	Class # of Compound
17	20	Compound #
21	21	Ion #
23	24	Ordinal # of Standard within Record
26	27	ID # of Standard within Record

The fields in columns 11-21 locate the entry as with the ASTD card. Ordinal number of the standard within the entry (columns 23-24) is used as a check against the standard ID to ensure that the correct standard reference is deleted.

Beginning Column	Ending Column	
1	4	CRMR
11	14	Record # for Compound
15	16	Class # for Compound
17	20	Compound #
21	21	Ion #
23	24	Ordinal # for Standard on Report
26	27	ID # of Standard on Report
31	33	Standard Ion Mass #1
35	39	RMR #1
41	43	Standard Ion Mass #2
45	49	RMR #2

The CRMR control card information is meant to be taken from the output of REPORT. The EDIT program uses the compound #, class #, and ion # to locate the entry in the data base and the record # as a double check. The standard ordinal #, standard ID # and standard ion mass are used to locate the correct standard ion mass on the data base entry matches the mass entered in card columns 31-33, then the data base RMR for that standard is replaced by contents of card columns 35-39. Likewise, if the second standard ion mass on the data base entry matches the mass entered in card columns 41-43 the data base RMR for that standard is replaced by the contents of card columns 45-49. Leaving a standard ion mass field blank will result in no RMR change regardless of the contents of the corresponding RMR field.

The ASTD card is used to add standard references to existing entries in both the analyte and standard files and thereby enter RMR information of existing entries entries versus newly added standards to the data base.


Old
MASQNT
File
Unsorted
Control
Cards
Sort in Ascending
Order on
Cols 15-16
(Class #)
Cols 17-20
(Compound #)
Col 21 (Ion #)
EDIT
Program
Sorted
Card Image
EDIT Changes
Edit
MASQ
File

Steps for EDIT Program

ADD

The program ADD is used to add new compounds to the MASQNT data base. ADD reads in the new compounds from card images on unit 1, reads the old MASQNT file from unit 7, and writes the new MASQNT file with added entries to unit 8. Before the new MASQNT file created by ADD can be used by the MASQNT program, it must be sorted in order of ascending class number (columns 91-92) and in order of ascending compound number (columns 87-90) within class #. It is strongly recommended that any new additions to the MASQNT files be proofed by use of the REPORT program before they are used as input data for MASQNT. Like DELETE and EDIT, each run of ADD is tentative until the old file is deleted and the new file is renamed to the old file name.

The ADD program recognizes three kinds of control cards: The ADD card which supplies numeric information on the compound being added, the NAME card which supplies the name of the compound being added, and the STD card which supplies information on the RMR's and ion masses for each entry. The card image input to ADD for each compound consists of first an ADD card, followed by a NAME card, and however many STD cards were specified in the fields for number of ions and number of standard on the ADD card. The program checks for proper sequence of ADD-NAME-STD cards and for the proper number of STD cards following the ADD and NAME cards and issues an appropriate error message if there is a discrepancy.

The items for the ADD card with their respective columns are as follows:

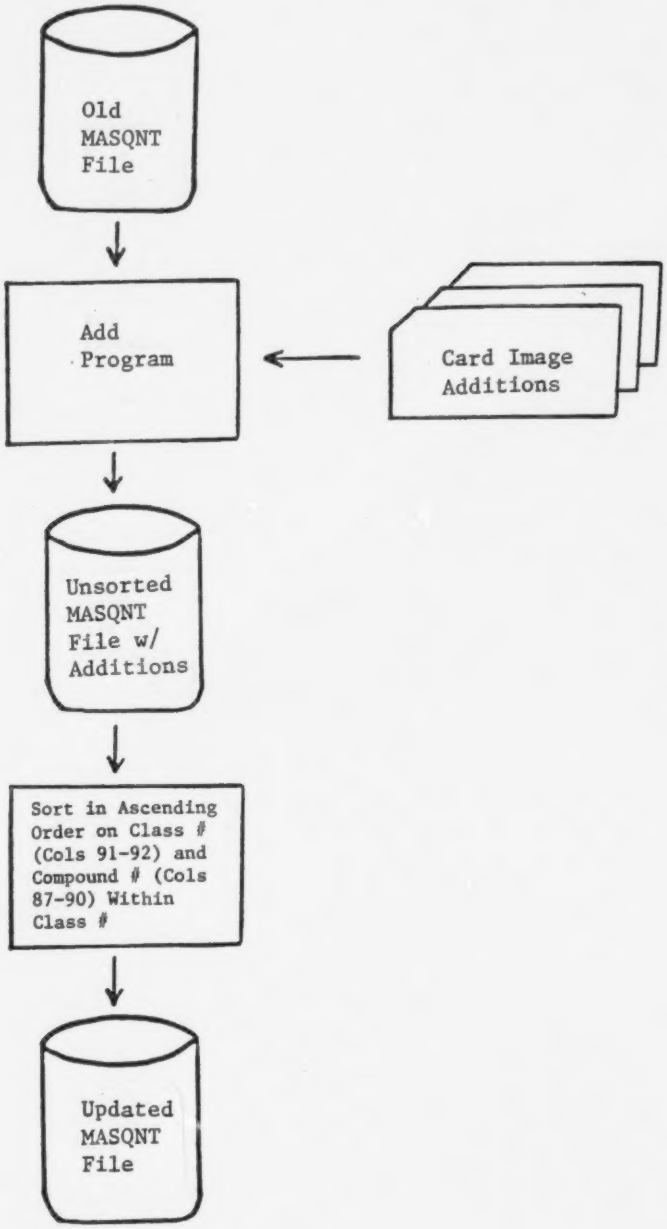
When adding compounds to the data base new compounds ID's have to be assigned. Each new entry must have a compound ID number assigned to it. It is crucial that the compound ID's (columns 11-12 of the STD card) be assigned consistently. The compound numbers must fulfill two requirements: A range requirement and uniqueness within compound class. The compound ID numbers must be within the following ranges:

External Standards	1-49
Internal Standards	51-99
Analytes	100-999

The types for standards must also follow the conditions:

Internal Standards Type = 2
External Standards Type = 1
Analytes Type = 3

Whether making additions to the standard file or to the analyte file, the output file generated by ADD must be sorted in order of increasing class number (columns 91-92) and in order of increasing compound number (columns 87-90) within class number. After being sorted the file should have new entries verified by the REPORT program before the new file is used by MASQNT.


Old MASQNT File
Add Program
Card Image Additions
Unsorted MASQNT File w/ Additions
Sort in Ascending Order on Class # (Cols 91-92) and Compound # (Cols 87-90) Within Class #
Updated MASQNT File

Steps for ADD Program

Mass Quantitation Data Entry

ADD	NO IONS	NO STDS	CLASS NUMBER	TYPE	ION MASS NUMBER 1	ION MASS NUMBER 2	MOLECULAR WEIGHT	RECOVERY	COMPOUND NUMBER	
A D D										

NAME	COMPOUND NAME
N A M E	

STD	ION NO.	SEQ. NO.	STD ID	STD TYPE	STD MASS NUMBER 1	STD RMR NUMBER 1	STD MASS NUMBER 2	STD RMR NUMBER 2
S T D	1	1						
S T D	1	2						
S T D	1	3						
S T D	1	4						
S T D	1	5						
S T D	1	6						
S T D	1	7						
S T D	1	8						
S T D	1	9						
S T D	1	1 0						
S T D	1	1 1						
S T D	1	1 2						
S T D	1	1 3						
S T D	1	1 4						
S T D	1	1 5						
S T D	1	1 6						
S T D	2	1						
S T D	2	2						
S T D	2	3						
S T D	2	4						
S T D	2	5						
S T D	2	6						
S T D	2	7						
S T D	2	8						
S T D	2	9						
S T D	2	1 0						
S T D	2	1 1						
S T D	2	1 2						
S T D	2	1 3						
S T D	2	1 4						
S T D	2	1 5						
S T D	2	1 6						

Figure C-1. Flow Chart of Master Scheme Software

November, 1980

Glossary

PPM = Parts per Million

PPB = Parts per Billion

FACT = Factor

SPS = System Performance Standards

VOL = Volume

IS = Internal Standard

XS = External Standard

RRT = Relative Retention Time

WT = Weight

UNK = Unknown

MW = Molecular Weight

SR = System Response

RMR = Relative Molar Response

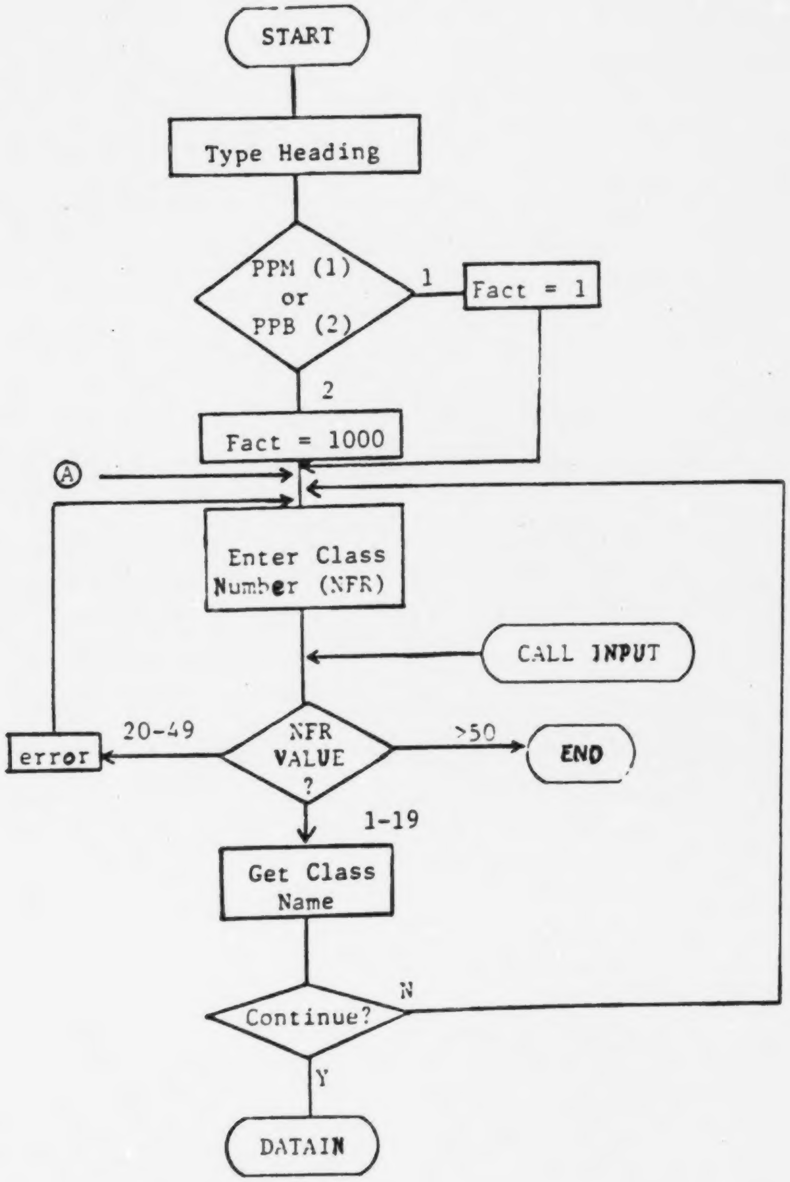
FOR = Forward

BACK = Backward

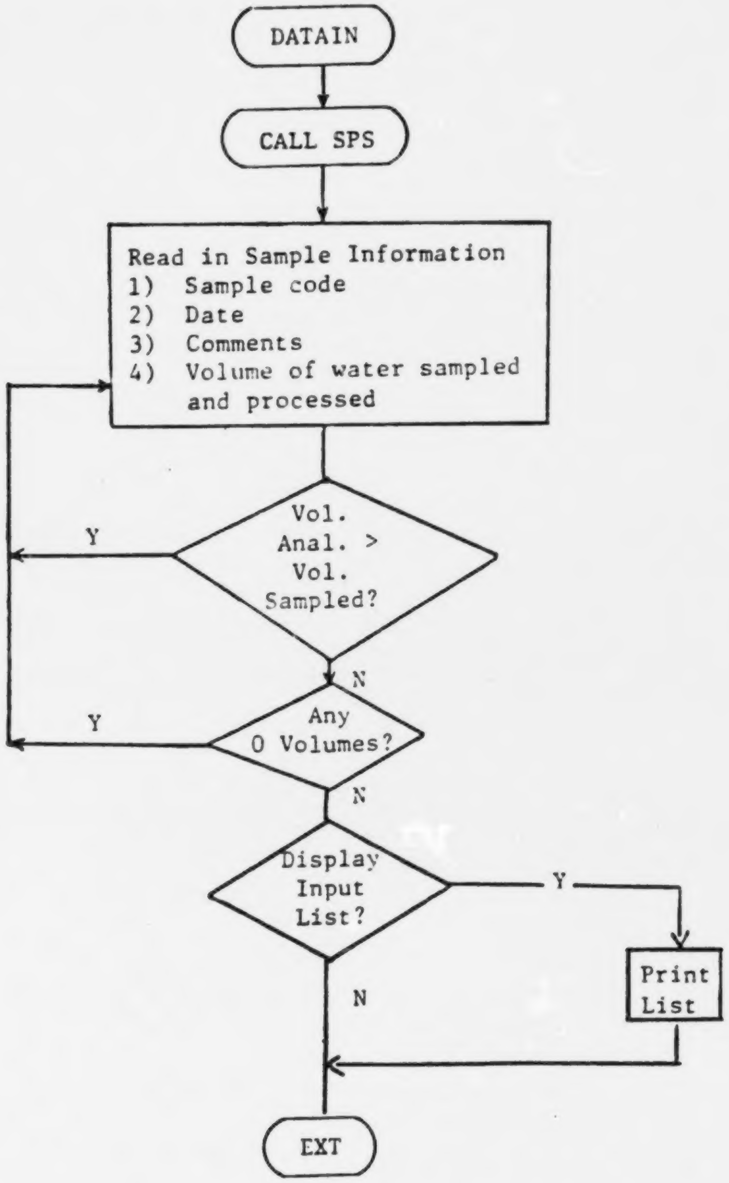
(continued)

Flow Chart of Master Scheme Software

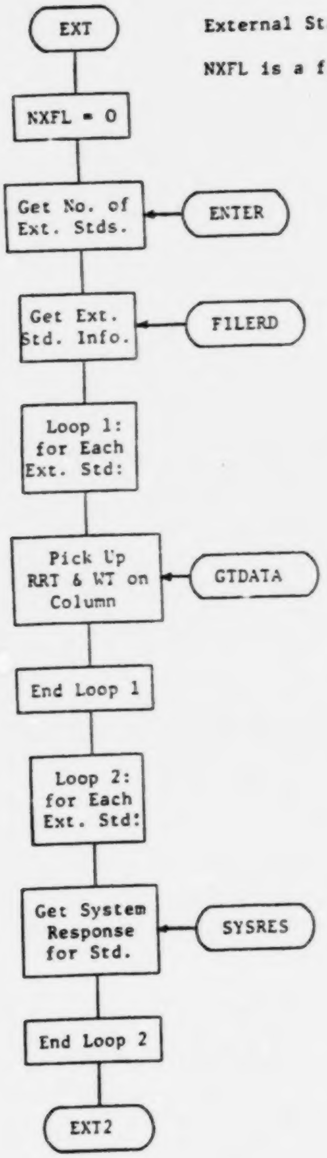
November, 1980


START
Type Heading
PPM (1)
or
PPB (2)
1
Fact = 1
2
Fact = 1000
A
Enter Class
Number (NFR)
CALL INPUT
20-49
error
NFR
VALUE
?
>50
END
1-19
Get Class
Name
N
Continue?
Y
DATAIN

(continued)


DATAIN
CALL SPS
Read in Sample Information
1) Sample code
2) Date
3) Comments
4) Volume of water sampled and processed
Vol. Anal. > Vol. Sampled?
Y
N
Any 0 Volumes?
Y
N
Display Input List?
Y
N
Print List
EXT

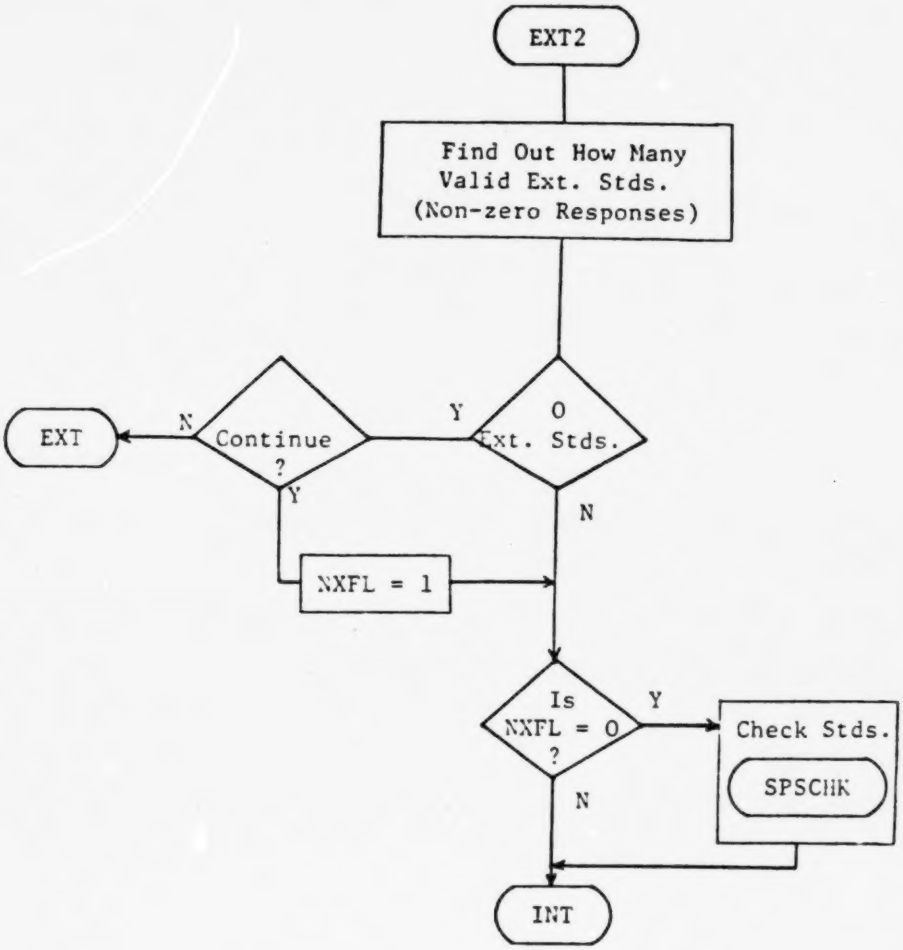
(continued)


EXT
NXFL = 0
Get No. of Ext. Stds.
ENTER
Get Ext. Std. Info.
FILERD
Loop 1: for Each Ext. Std:
Pick Up RRT & WT on Column
GTDATA
End Loop 1
Loop 2: for Each Ext. Std:
Get System Response for Std.
SYSRES
End Loop 2
EXT2

External Standard Information

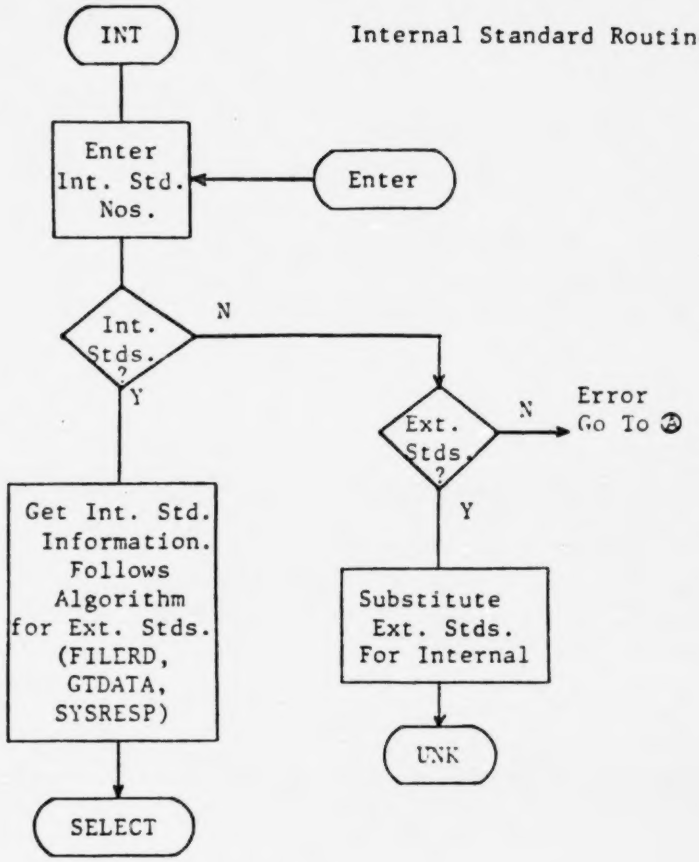
NXFL is a flag indicating XS.

(continued)

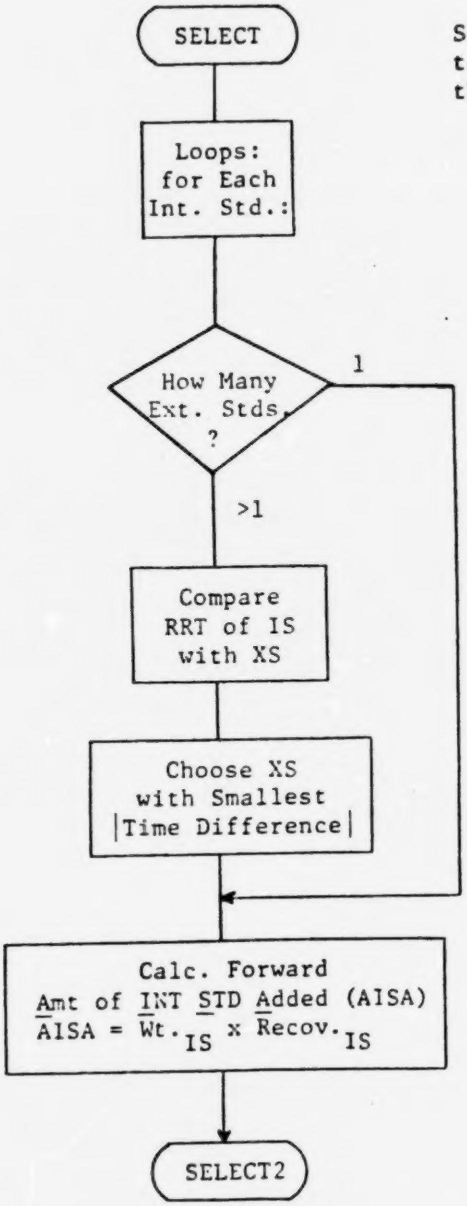

EXT2
Find Out How Many Valid Ext. Stds. (Non-zero Responses)
0 Ext. Stds.
Y
N
Continue ?
N
Y
EXT
NXFL = 1
Is NXFL = 0 ?
Y
N
Check Stds.
SPSCHK
INT

(continued)

Internal Standard Routine

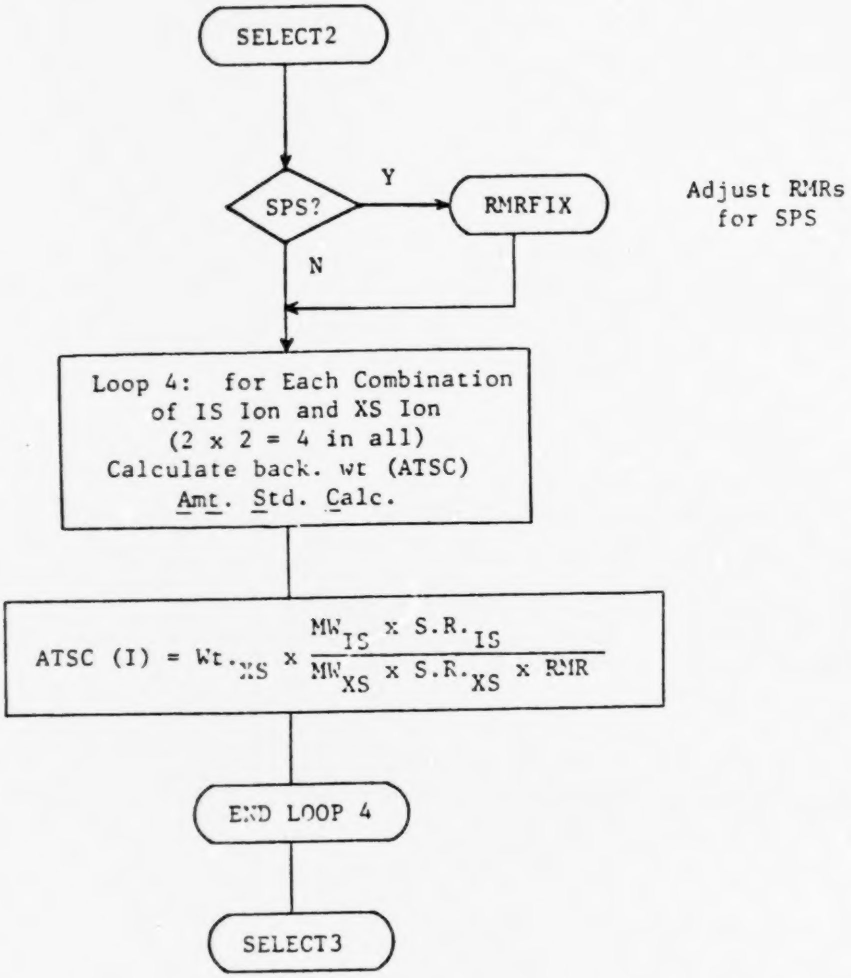

INT
Enter Int. Std. Nos.
Enter
Int. Stds. ?
N
Y
Ext. Stds. ?
N
Error Go To ③
Y
Get Int. Std. Information. Follows Algorithm for Ext. Stds. (FILERD, GTDATA, SYSRESP)
Substitute Ext. Stds. For Internal
UNK
SELECT

(continued)

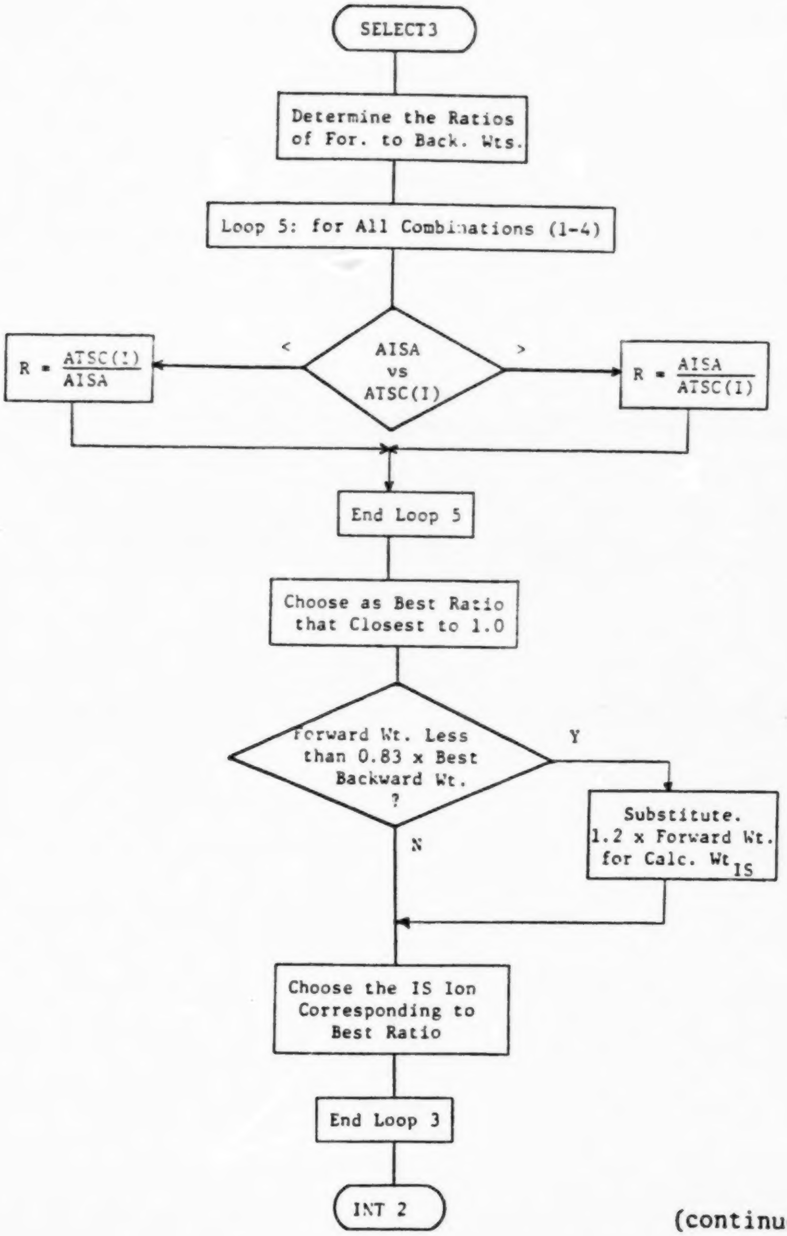

SELECT
Loops: for Each Int. Std.:
How Many Ext. Stds. ?
1
>1
Compare RRT of IS with XS
Choose XS with Smallest |Time Difference|
Calc. Forward Amt of INT STD Added (AISA)
AISA = Wt.$_{IS}$ x Recov.$_{IS}$
SELECT2

Select which Int. Std. ion to use if data for more than one ion is available.

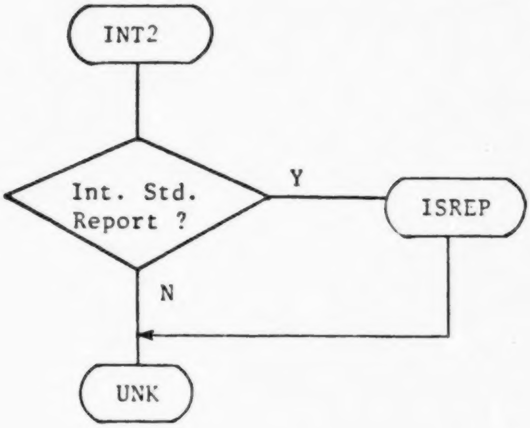
(continued)


SELECT2
SPS?
Y
N
RMRFIX
Adjust RMRs for SPS
Loop 4: for Each Combination of IS Ion and XS Ion (2 x 2 = 4 in all) Calculate back. wt (ATSC) Amt. Std. Calc.
$\text{ATSC (I)} = \text{Wt.}_{XS} \times \frac{MW_{IS} \times S.R._{IS}}{MW_{XS} \times S.R._{XS} \times RMR}$
END LOOP 4
SELECT3

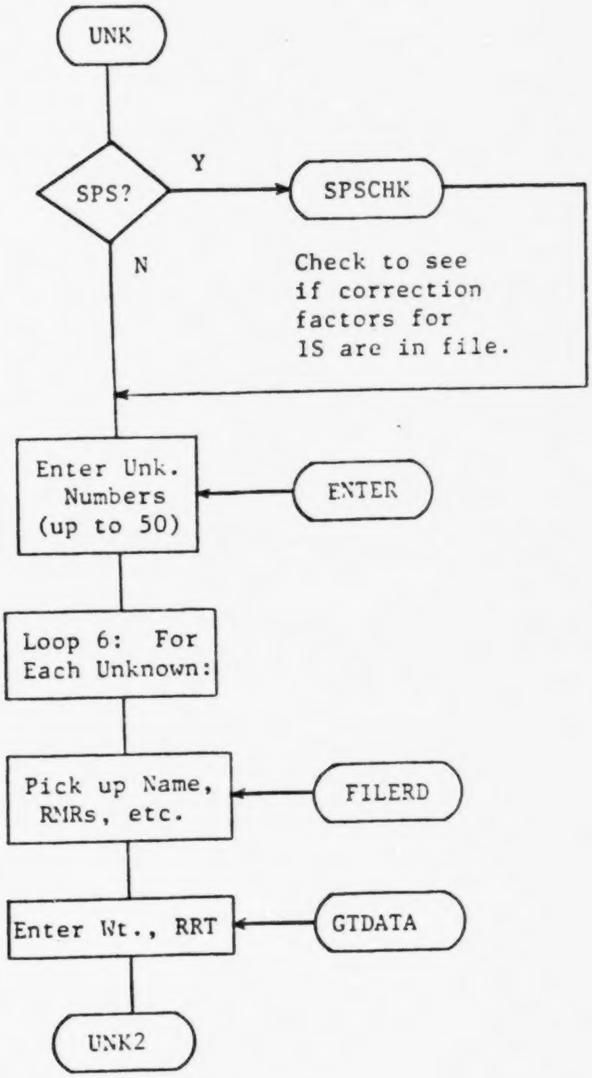
(continued)


SELECT3
Determine the Ratios of For. to Back. Wts.
Loop 5: for All Combinations (1-4)
AISA vs ATSC(I)
<
>
R = ATSC(I) / AISA
R = AISA / ATSC(I)
End Loop 5
Choose as Best Ratio that Closest to 1.0
Forward Wt. Less than 0.83 x Best Backward Wt. ?
Y
N
Substitute. 1.2 x Forward Wt. for Calc. Wt IS
Choose the IS Ion Corresponding to Best Ratio
End Loop 3
INT 2

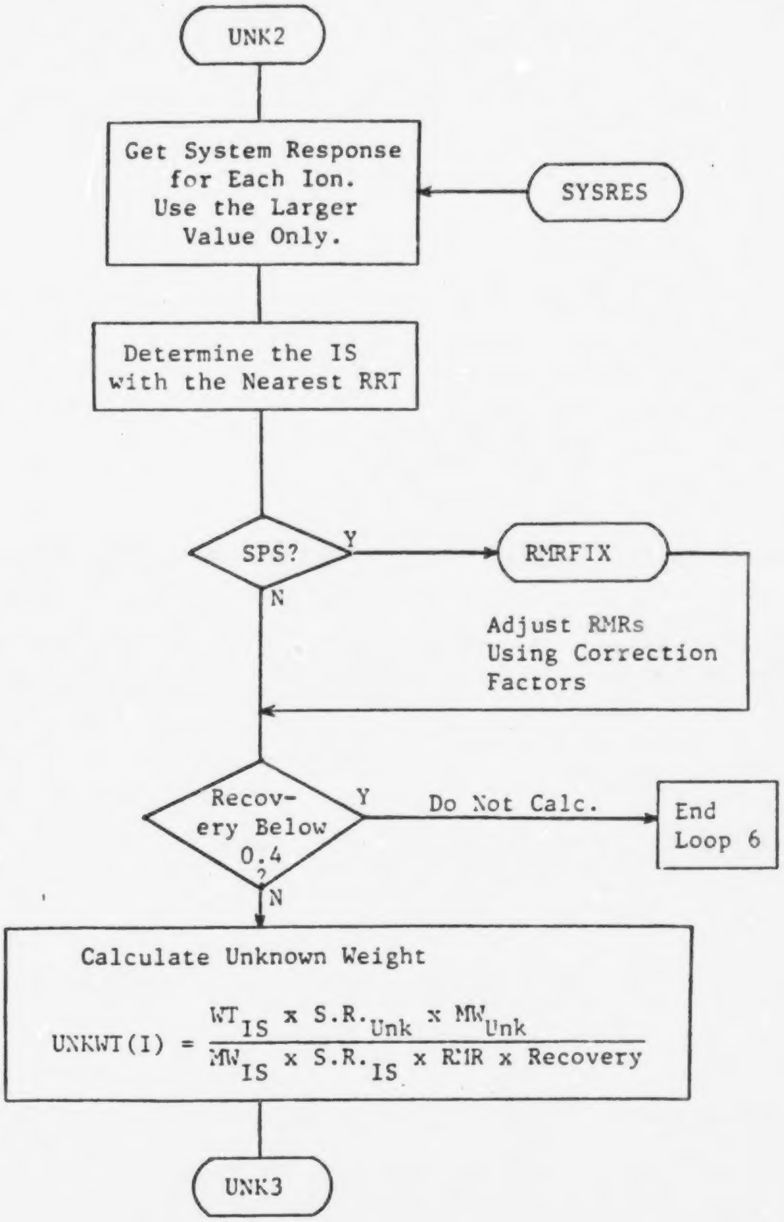
(continued)


INT2
Int. Std. Report ?
Y
ISREP
N
UNK

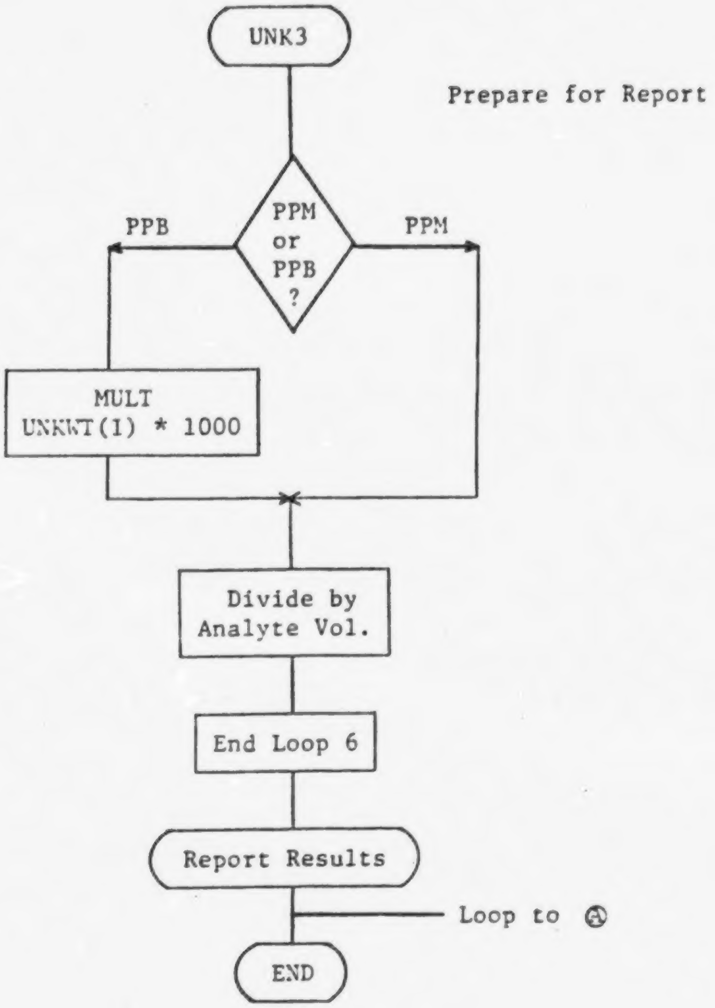
(continued)


UNK
SPS?
Y
N
SPSCHK
Check to see if correction factors for IS are in file.
Enter Unk. Numbers (up to 50)
ENTER
Loop 6: For Each Unknown:
Pick up Name, RMRs, etc.
FILERD
Enter Wt., RRT
GTDATA
UNK2

(continued)

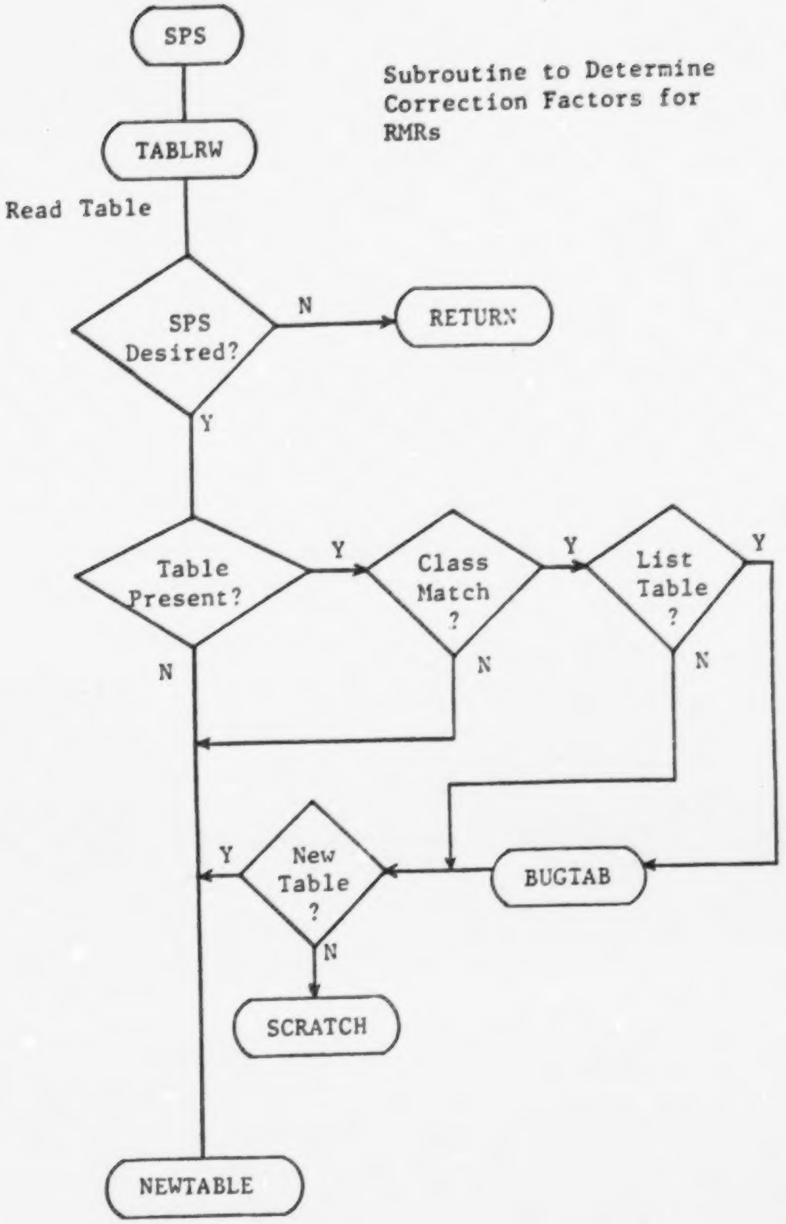

UNK2
Get System Response for Each Ion. Use the Larger Value Only.
SYSRES
Determine the IS with the Nearest RRT
SPS?
Y
N
RMRFIX
Adjust RMRs Using Correction Factors
Recovery Below 0.4 ?
Y
Do Not Calc.
End Loop 6
N
Calculate Unknown Weight
UNKWT(I) = $\frac{WT_{IS} \times S.R._{Unk} \times MW_{Unk}}{MW_{IS} \times S.R._{IS} \times RMR \times Recovery}$
UNK3

(continued)

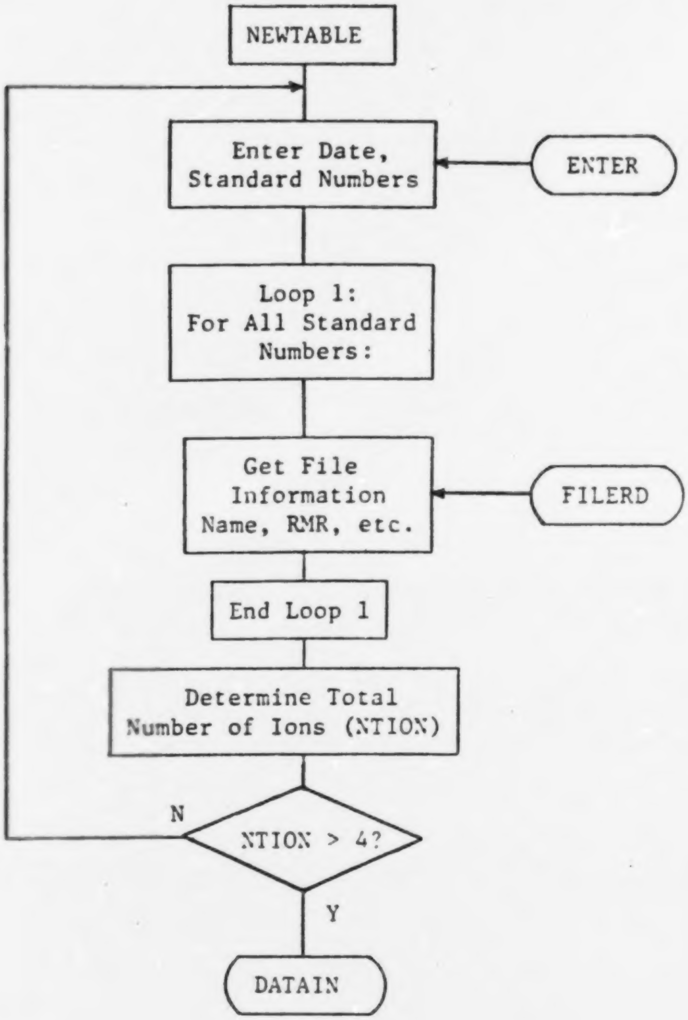

UNK3
Prepare for Report
PPM or PPB ?
PPB
PPM
MULT UNKWT(I) * 1000
Divide by Analyte Vol.
End Loop 6
Report Results
Loop to Ⓐ
END

(continued)

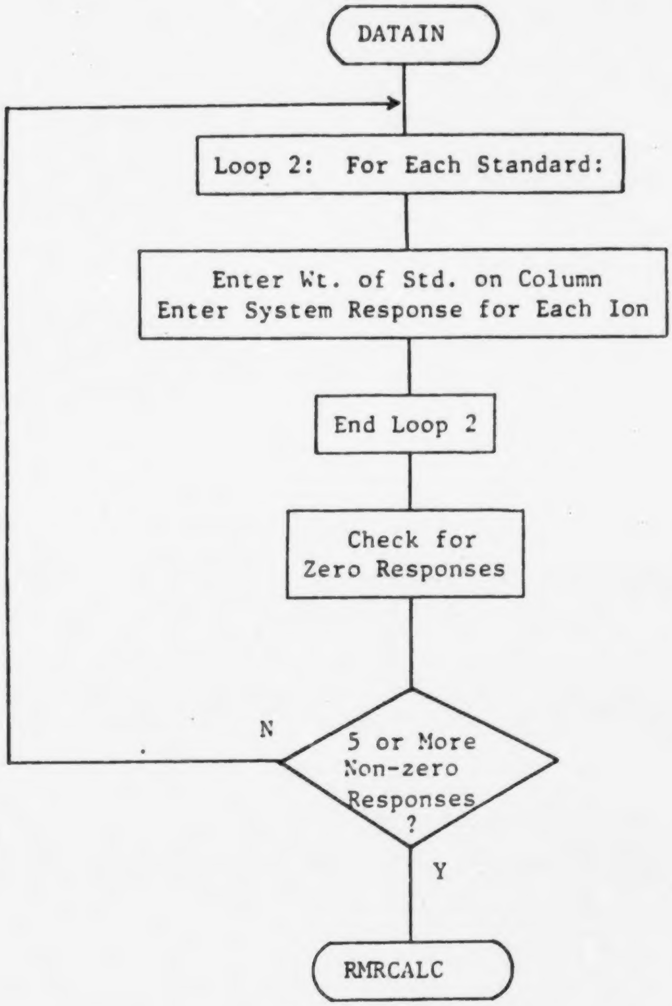
Subroutine to Determine Correction Factors for RMRs


SPS
TABLRW
Read Table
SPS Desired?
N
RETURN
Y
Table Present?
Y
Class Match ?
Y
List Table ?
Y
N
N
N
Y
New Table ?
BUGTAB
N
SCRATCH
NEWTABLE

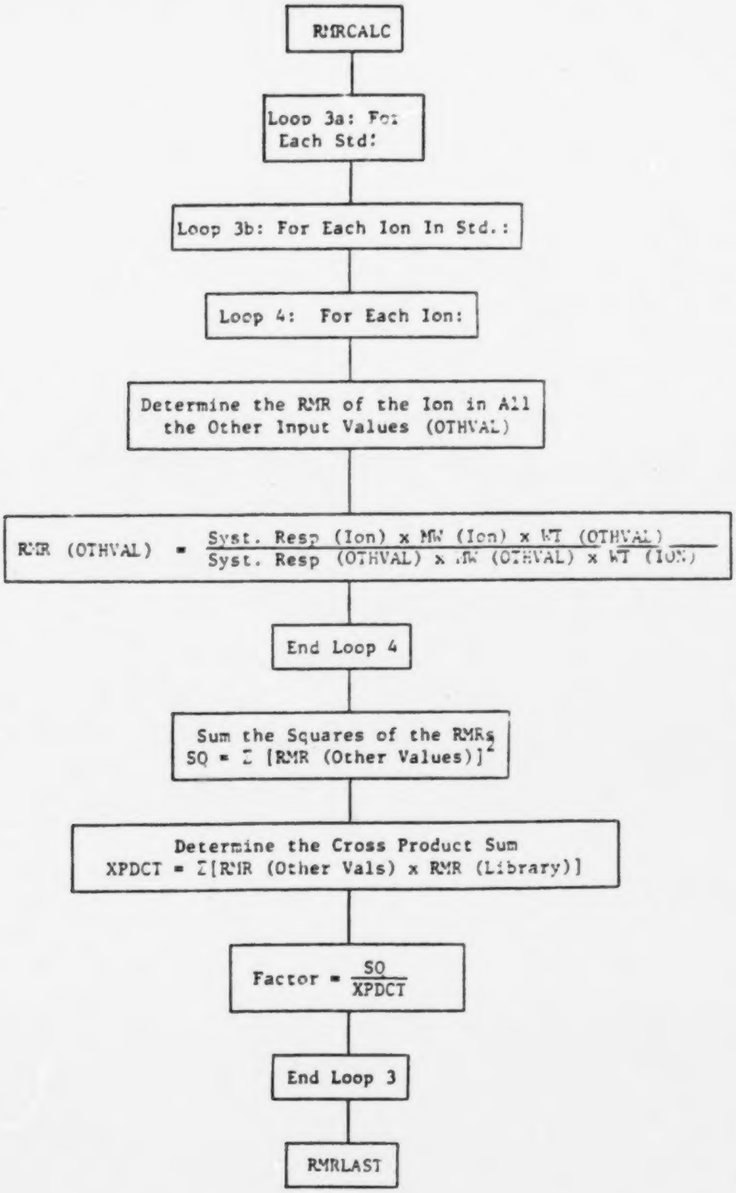
(continued)


NEWTABLE
Enter Date, Standard Numbers
ENTER
Loop 1: For All Standard Numbers:
Get File Information Name, RMR, etc.
FILERD
End Loop 1
Determine Total Number of Ions (NTION)
N
NTION > 4?
Y
DATAIN

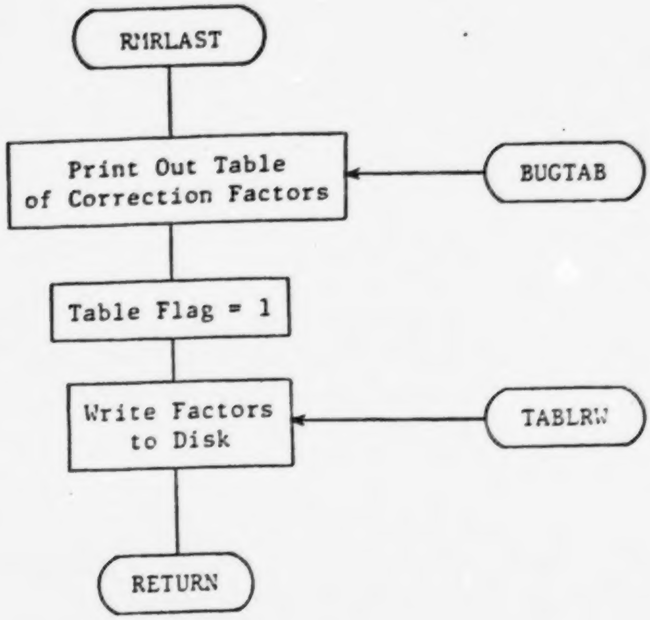
(continued)

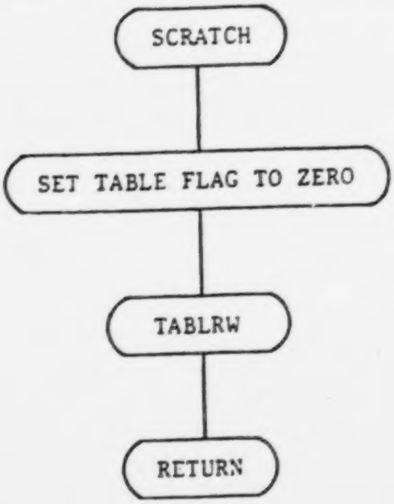

DATAIN
Loop 2: For Each Standard:
Enter Wt. of Std. on Column
Enter System Response for Each Ion
End Loop 2
Check for
Zero Responses
N
5 or More
Non-zero
Responses
?
Y
RMRCALC

(continued)


RMRCALC
Loop 3a: For Each Std:
Loop 3b: For Each Ion In Std.:
Loop 4: For Each Ion:
Determine the RMR of the Ion in All the Other Input Values (OTHVAL)
RMR (OTHVAL) = Syst. Resp (Ion) x MW (Ion) x WT (OTHVAL) / Syst. Resp (OTHVAL) x MW (OTHVAL) x WT (ION)
End Loop 4
Sum the Squares of the RMRs
SQ = Σ [RMR (Other Values)]²
Determine the Cross Product Sum
XPDCT = Σ[RMR (Other Vals) x RMR (Library)]
Factor = SQ / XPDCT
End Loop 3
RMRLAST

(continued)


RMRLAST
Print Out Table of Correction Factors
BUGTAB
Table Flag = 1
Write Factors to Disk
TABLRW
RETURN


SCRATCH
SET TABLE FLAG TO ZERO
TABLRW
RETURN